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DTU Environment
Department of Environmental Engineering

PhD Thesis
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The synopsis part of this thesis is available as a pdf-file for download from the DTU research database ORBIT: http://www.orbit.dtu.dk


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# Preface

This thesis is based on the work carried out at the Department of Environmental Engineering at the Technical University of Denmark from October 2010 to January 2014. This thesis was prepared as part of the Storm and Wastewater Informatics (SWI) project (http://www.swi.env.dtu.dk) and was funded by the Danish Council for Strategic Research, Programme Commission on Sustainable Energy and Environment, the Technical University of Denmark and the utility companies HOFOR, Lynettefællesskabet, Spildevandscenter Avedøre and Aarhus Vand. The research was performed under the main supervision of Associate Professor Benedek G. Plósz (DTU Environment), and co-supervision of Professor Peter S. Mikkelsen (DTU Environment), Lars Yde (DHI, Singapore), and Associate Professor Michael R. Rasmussen (Aalborg University).

The thesis is organized in two parts: the first part puts into context the findings of the PhD in an introductive review; the second part consists of the papers listed below. These will be referred to in the text by their paper number written with the Roman numerals **I-IV**.

**I** **Ramin, E.**, Flores Alsina, X., Sin, G., Gernaey, K.V., Jeppsson, U., Mikkelsen, P.S., and Plósz, B.G. (2014). Influence of selecting secondary settling tank sub-models on the calibration of WWTP models – A global sensitivity analysis using BSM2. *Chemical Engineering Journal*. **241**: 28-34.

**II** **Ramin, E.**, Sin, G., Mikkelsen, P.S., and Plósz, B.G. (2014). Significance of settling model structures and parameter subsets in modelling WWTPs under wet-weather flow and filamentous bulking conditions. *Submitted manuscript*.

**III** **Ramin, E.**, Wágner, D.S., Yde, L., Binning, P.J., Rasmussen, M.R., Mikkelsen, P.S., and Plósz, B.G. (2014). A new settling velocity and rheological model for secondary settling tank modelling. *Submitted manuscript*.

**IV** **Ramin, E.**, Wágner, D.S., Szabo, P., Dechesne, A., Smets, B.F, and Plósz, B.G. (2014). Impact of filamentous microbial community characteristics on activated sludge settling and rheological behaviour – measurements and numerical modelling. *Manuscript in preparation*.

In addition, the following co-authored publications were also established during this PhD study, but are not included in this thesis:

- Wágner, D.S., **Ramin, E.**, Dechesne, A., Smets, B.F., Szabo, P., and Plósz, B.G. (2014). Impact of filamentous bacteria on the settling velocity and rheology of activated sludge. *Manuscript in preparation*.

- Valverde-Pérez, B., **Ramin, E.**, Smets, B.F., and Plósz, B.G. (2014). An innovative enhanced biological nutrient recovery activated sludge system – evaluation of the combined operation with a photobioreactor. *Manuscript in preparation*.

In this online version of the thesis, the articles are not included but can be obtained from electronic article databases e.g. via www.orbit.dtu.dk or on request from DTU Environment, Technical University of Denmark, Miljøvej, Building 113, 2800 Kgs. Lyngby, Denmark, reception@env.dtu.dk.

This PhD study also contributed to international conferences with the following proceeding papers:

1 **Ramin E.**, Sin G., Mikkelsen P.S., Plosz B.G. Significance of uncertainties derived from settling tank model structure and parameters on predicting WWTP performance–a global sensitivity analysis study. 8th IWA Symposium on Systems Analysis and Integrated Assessment, Watermatex, San Sebastian, Spain, 20–22 June 2011.

2 **Ramin, E.**, Flores Alsina, X., Sin, G., Gernaey, K.V., Jeppsson, U., Mikkelsen, P.S., and Plósz, B.G. (2012). Relative importance of secondary settling tank models in WWTP simulations: A global sensitivity analysis using BSM2. 6th International Congress on Environmental Modelling and Software, iEMSs, Leipzig, Germany, 1–5 July 2012.

3 Smets, B.F., Pellicer i Nàcher, C., B., Jensen, M.M., **Ramin, E.**, Plósz, B.G., Domingo Felez, C., Mutlu, A.G., Scheutz, C., Thamdrup, B., Chandran, K., Sin, G., Lemaire, R., and Kuypers, M. (2013). Modelling N2O dynamics in the engineered N cycle: observations, assumptions, knowns, and unknowns. 3rd international conference on Nitrification, ICON3, Tokyo, Japan, 2–5 September 2013.

4 **Ramin, E.**, Wágner, D.S., Yde, L., Rasmussen, M.R., Smets, B.F., Mikkelsen, P.S., and Plósz, B.G. (2014). Modelling the impact of filamentous bacteria abundance in a secondary settling tank: CFD sub-models optimization using long-term experimental data. 4th international seminar on wastewater treatment modelling, WWTmod2014, Belgium, Spa, 28 March–2 April 2014.

Acknowledgements

This PhD study could have not been accomplished without the great contributions that I received in the last three years.

First, I would like to thank my supervisor Associate Professor Benedek Plósz for his constant guidance and enthusiasm. I would also like to thank my co-supervisors Prof. Peter Steen Mikkelsen for his valuable and sincere feedbacks, Lard Yde for his guidance on computational fluid dynamics modelling, particularly during my external stay at DHI Singapore, and Associate Professor Michael Rasmussen for his advice on hydrodynamics modelling.

I would like to thank all the utilities and companies involved in the Storm Wastewater Informatics (SWI) project for their financial support. I would also like to thank Dr. Anitha Sharma, coordinator of the SWI project, for her technical support.

I am grateful to Professor Hans-Jørgen Albrechtsen, the head of Urban Water Engineering section at DTU Environment, for his supervision on my overall progress during my PhD study, and to the UrbanWaterTech graduate school for the possibility of interacting with other researchers at scientific seminars.

During my PhD studies, I had the honour to collaborate with Associate Professor Gürkan Sin, Dr. Xavier Flores-Alsina, Professor Krist Gernaey, Associate Professor Peter Szabo, Dr. Arnaud Dechesne and Professor Barth Smets. I greatly appreciated the valuable enriching experience of working with them. I would like to especially thank Dorottya Wágner for her hard work and supportive collaboration during the last year of my PhD. I would also like to thank Borja Valverde-Pérez for involving me in his research.

Working at DTU Environment was a great experience. I would like to thank all of my colleagues and friends for making my work place comfortable, motivating, and fun. I would like to give special thanks to Anne-Margrethe Harsting for her help with administrative issues.

Additionally I would like to extend my thanks and appreciations to my dear friends Fabio, Yoshi, Carson, Gizem, Suzi, Pau, Carles, Gamze and all of the Haydi Koçum people, with whom I shared nice moments that will always be in my memory.

There will never be enough words to thank my family for their love and support.

# Summary

Secondary settling tanks (SSTs) are the most hydraulically sensitive unit operations in wastewater treatment plants (WWTPs). Performance of SSTs influences the solids inventory in the activated sludge unit and consequently impacts the biological treatment efficiency. Moreover, SSTs limit the maximum permissible flow rate entering the WWTPs during wet-weather conditions. Therefore, modelling the dynamics in the SSTs is an essential part of integrated sewer- WWTP modelling for the purpose of optimization and control, specifically under wet-weather conditions. One-dimensional (1-D) SST models with first-order type equations are widely used among researches and practitioners for dynamic WWTP simulations. Several drawbacks of the first-order models have however been reported in the literature, which have led to the development of more advanced second-order 1-D SST models.

Unfortunately, the second-order models have not yet found their way into practice. This thesis aims at encouraging a broader application of second-order 1-D SST models by assessing their significance for WWTP modelling by means of global sensitivity analysis (GSA). Moreover, laboratory and numerical (computational fluid dynamics, CFD) tools were developed for the identification and calibration of the settling sub-model in the SST models. The developed CFD tool is a potential tool for the development of a more mechanistic based flow (and design) dependent hydraulic sub-model in the second-order 1-D SST.

In this thesis, a rigorous comparative evaluation of the first- and second-order SST models in WWTP modelling was performed by means of GSA. In the first GSA study using the Benchmark Simulation Model No. 2 with first- and second-order SST models, the settling parameters were included in the sensitivity analysis. Interestingly, the settling parameters were found to be among the most influential parameters for predicting the WWTP performance in terms of biogas production and quality of treated water. Importantly, it was observed that the choice of 1-D SST type model influences the sensitivity measures of the parameters and consequently result in different parameter sub-sets for the calibration of WWTP models. Furthermore, the limitations of first-order SST models with relevance to the calibration of WWTP models were discussed.

In the second GSA study of this thesis, the aim was to supplement the protocol recently published by the International Water Association on good modelling practice for activated sludge systems with practical findings on the

calibration of 1-D SST models for dynamic WWTP simulations under ideal and non-ideal flow (dry- or wet-weather) and settling (good settling and/or bulking) boundary conditions. The Benchmark simulation model No. 1 in combination with first- and second-order 1-D SST models was used. An assessment was performed on the sensitivity of WWTP model outputs to uncertainties intrinsic to 1-D SST model structures and parameters under different boundary conditions imposed to WWTP simulation models. Further, the relative sensitivity to these uncertainties indicated potential parameter subsets for WWTP model calibration and the optimal choice of 1-D settling model structure under the different boundary conditions. Importantly, the hydraulic parameters in the second-order 1-D SST model were found significant under dynamic wet-weather flow conditions. The results of this study illustrated the advantages of second-order 1-D SST models for dynamics WWTP simulations under wider flow and bulking conditions, and furthermore, highlighted the necessity of developing a more mechanistic based flow-dependent hydraulic sub-model in second-order 1-D SST models in the future.

A significant part of the thesis was dedicated to the development of a CFD model of a circular conical SST with the open source OpenFOAM CFD toolbox. The focus was mainly on identifying the settling and rheology sub-models using data obtained from laboratory batch experiments. A simple, novel settling column experimental set-up was developed to evaluate the accuracy of the state-of-the-art settling velocity models. For calibration the Bayesian optimization method $DREAM_{(ZS)}$ was used. Consequently, a new settling velocity model, including hindered, transient and compression settling, was developed. In addition, a rheology model of activated sludge was selected and calibrated to high quality rheological measurements from the optimized batch experiments. New correlations between rheology model parameters and sludge concentration were identified. A 2-D axisymmetric CFD model of a circular SST containing the new settling velocity and rheology sub-models were validated with full-scale measurements. Finally, it was shown that the representation of compression settling in the CFD model greatly influences the prediction of sludge distribution in the SSTs. The validated CFD model was further used in the last study of this thesis to model the impact of filamentous bulking on the sludge distribution and transport in SSTs by calibrating the rheology and settling sub-models to measurements of sludge with high and low filamentous bacteria content.

# Dansk sammenfatning

Efterklaringstanke (eng: secondary settling tanks, SSTs) er de mest hydraulisk følsomme enhedsoperationer i spildevands renseanlæg. Ydeevnen af efterklaringstanke påvirker fordelingen af slam i anlægget og påvirker dermed også effektiviteten af den biologiske behandling. Desuden begrænser efterklaringstanke den maksimalt tilladte flowrate til renseanlæg under regnvejr. Derfor er modellering af dynamikken i efterklaringstanke en væsentlig del af modelleringen af integrerede systemer bestående af afløbssystemer og renseanlæg, med henblik på optimering og styring særligt under regnvejr. Éndimensionale (1-D) SST modeller med første-ordens ligninger er meget udbredte blandt forskere og praktikere til dynamisk simulering af renseanlæg. Der er i litteraturen imidlertid rapporteret adskillige ulemper ved første-ordens modellerne, hvilket har ført til udvikling af mere avancerede anden-ordens 1-D SST modeller.

Desværre anvendes anden-ordens modellerne endnu ikke i praksis. Denne afhandling har til formål at tilskynde til en bredere anvendelse af anden-ordens 1-D SST modeller ved at vurdere deres betydning for modellering af renseanlæg ved hjælp af global sensitivitetsanalyse (GSA). Desuden blev laboratorie metoder og numeriske beregningsværktøjer (Computational Fluid Dynamics CFD) udviklet til identifikation og kalibrering af bundfældnings-submodellen i SST modellerne. Det udviklede CFD værktøj er et potentielt redskab til udvikling af en mere mekanistisk baseret flow- og designafhængig hydrauliske sub-model i anden ordens 1-D SST modeller.

I denne afhandling blev GSA anvendt til at udføre en stringent sammenligning og evaluering af første- og anden-ordens SST modeller i forbindelse med modellering af renseanlæg. I den første GSA undersøgelse med Benchmark simuleringsmodel nr. 2 i kombination med første- og anden-ordens SST modeller, blev bundfældningsparametrene inkluderet i sensitivitetsanalysen. Dette viste, at bundfældningsparametrene er blandt de mest betydningsfulde parametre ved beregning af renseanlægs ydeevne i form af biogasproduktion og kvalitet af det behandlede vand. En vigtig observation var, at valget af 1-D SST model påvirker parametrenes indflydelse og dermed resulterer i forskellige parameter sub-sæt til kalibrering af modeller for renseanlæg. Desuden blev begrænsningerne ved første-ordens SST modeller i forbindelse med kalibrering af modeller for renseanlæg diskuteret.

I den anden GSA undersøgelse i afhandlingen var formålet at supplere protokollen udgivet for nyligt af International Water Association om god modelleringspraksis for aktiv slam anlæg med praktiske anvisninger om kalibrering af 1-D SST modeller til dynamisk simulation af renseanlæg under ideale og ikke ideale randbetingelser for flow (tørvejr eller regnvejr) og bundfældning (god- og/eller ringe bundfældning). Benchmark simuleringsmodel nr. 1 blev brugt i kombination med første- og anden-ordens 1-D SST modeller. Der blev lavet en vurdering af følsomheden af renseanlægs modellers outputs overfor usikkerheder i 1-D SST modelstrukturer og -parametre under forskellige randbetingelser pålagt simuleringsmodellerne. Den relative følsomhed overfor disse usikkerheder indikerede endvidere potentielle parameter undergrupper til brug i modelkalibrering samt det optimale valg af 1-D bundfældnings modelstruktur under forskellige randbetingelser. En vigtigt pointe var at de hydrauliske parametre i anden ordens 1-D SST modellen blev fundet signifikante under dynamiske flowforhold under regn. Resultaterne af denne undersøgelse viser fordelene ved anden ordens 1-D SST modeller til dynamisk simulering af renseanlæg under varierende flow og bundfældningsbetingelser, og de understreger desuden nødvendigheden af fremover at udvikle en mere mekanistisk baseret flowafhængig hydraulisk sub-model i anden ordens 1-D SST modeller.

En væsentlig del af afhandlingen var dedikeret til udviklingen af en CFD model af en cirkulær konisk SST med open-source software pakken OpenFOAM. Fokus var hovedsageligt på at identificere bundfældnings og rheologi delmodeller ved brug af data fra laboratorie batch eksperimenter. En simpel, ny forsøgsopstilling med en enkel bundfældnings kolonne blev udviklet for at vurdere nøjagtigheden af ”state-of-the-art” modeller for bundfældnings hastighed. Den Bayesianske optimeringsmetode $\mathrm{DREAM}_{(\mathrm{ZS})}$ blev anvendt til kalibrering. Dermed blev der udviklet en ny bundfældnings-hastighedsmodel, der inkluderede hindret, transient og kompressions bundfældning. Desuden blev en rheologi model for aktivt slam udvalgt og kalibreret til rheologi målinger af høj kvalitet fra de optimerede batch eksperimenter. Nye korrelationer mellem parametre i rheologi modeller og koncentrationen af slam blev identificeret. En 2-D aksesymmetrisk CFD model af en cirkulær SST, der indeholder de nye modeller for bundfældningshastigheder og rheologi, blev valideret ved brug af fuldskala målinger. Endelig blev det vist at indbygning af kompressions bundfældning i CFD modellen har stor betydning for forudsigelse af slamfordelingen i efterklaringstanke. Den validerede CFD model blev ydermere anvendt i afhandlingens sidste undersøgelse til at modellere påvirkningen af trådformede bakterier på fordelingen og transporten af slam i efterklaringstanke, ved at kalibrere rheologi- og bundfældningsmodellerne til målingerne på slam med højt og lavt indhold af trådformede bakterier.

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# 1 Introduction

## 1.1 Background and motivation

An increasing demand exists for the development of process models that predict the water quality in combined sewer- wastewater treatment systems under normal and wet-weather flow conditions, which can subsequently be used in optimization, online control and decision support. Under wet-weather flow conditions, the maximum permissible flow rate entering the wastewater treatment plants (WWTPs) is limited by the performance of secondary settling tanks, SSTs (Ekama et al., 1997). SSTs are located in the last stage of biological treatment in conventional activated sludge units to separate treated water from microbial sludge by gravity sedimentation.

Accurate prediction of the SST performance requires mechanistic models that can describe the internal interaction between the hydrodynamic and sludge distribution in the tank. On the other hand, the SST models, as part of an integrated sewer- WWTP model, benefit from having a relatively simple but robust model structure that requires less computation time and capacity. In this regard, one-dimensional (1-D) SST models are commonly used, to describe the vertical sludge profile in the tank by discretizing it into horizontal layers and considering the continuity of solid flux. These models can, therefore, give a reasonable approximation of the sludge balance and the sludge storage especially during wet-weather flow conditions. 1-D SST models have also been investigated for online use in integrated systems (Grijspeerdt et al., 1995; Bauwens et al., 1996).

In the last three decades, there have been significant advancements in 1-D modelling of SSTs. Since the development of Takács model (Takács et al., 1991) with first-order (hyperbolic) transport equation, second-order models that include an explicit dispersion term in the mass balance have been developed to overcome the numerical limitations of the first-order models (Chancelier et al., 1994; Diehl, 1996; Jeppsson and Diehl, 1996; Watts et al., 1996; Joannis et al., 1999; Plósz et al., 2007, 2011; De Clercq et al., 2008; David et al., 2009; Bürger et al., 2011). Furthermore, the second-order models with flow-dependent hydraulic sub-models (e.g. Plósz et al., 2007; Watts et al., 1996) have the advantage of simulating the hydraulics of settling tanks in wider flow conditions.

Nevertheless, second-order 1-D SST models have not yet found their way into the common WWTP modelling practice (Plósz et al., 2012). Global sensitivity analysis (GSA) can be used as an effective tool to evaluate the significance of first- and second-order SST model selection, by assessing the uncertainty derived from the SST model structure and parameters on the overall performance of WWTP models. 1-D SST models were subject to uncertainty analysis only in one study (Benedetti et al., 2012) using the first-order SST model. Due to differences in the model structure, the first and second-order 1-D SST models require different settings for their parameter values. As a result, selecting either of them would affect the sensitivity of WWTP model outputs to the settling parameters, and, consequently, their calibration. 1-D SST models are, after all, simplified models with lumped mathematical terms, accounting for the hydraulic processes that could not be described in one dimension. Therefore, the calibration of SST models depends on the settling and flow boundary imposed on the WWTP model. More specifically, by performing the sensitivity analysis of WWTP models, including second-order SST models with flow dependent (hydraulic) dispersion terms (e.g. Plósz et al., 2007), under ideal and non-ideal flow conditions, one can assess the significance of these type of SST models to WWTP simulations under wider flow conditions.

Computational fluid dynamics (CFD) models are proposed as useful tools to replace extensive field measurements for the optimization and calibration of 1-D SST models (De Clercq, 2003). In fact, CFD models have been used to generate data for developing more mechanistic-based hydraulic sub-models in second-order 1-D SST models (Plósz et al., 2007). To improve the prediction accuracy of the CFD models, research has mostly focused on optimizing the mathematical structure of the turbulence, and buoyant flow modelling components (Larsen, 1977; Adams and Rodi, 1990; Bretscher et al., 1992; Lakehal et al., 1999). At this time, despite significant advancements in research on the settling and rheological characteristics of activated sludge, their representation in CFD models of SSTs is not well-established. A few studies have incorporated optimized rheological models in the CFD models using laboratory experiments (De Clercq, 2003; Weiss et al., 2007). The other studies modified the rheological model parameters to obtain simulation results close to the observations (Dahl, 1993; Lakehal et al., 1999; Armbruster et al., 2001). In case of settling sub-models, the development of phenomenological sedimentation-consolidation theory has recently led to extensive studies on the compression settling behaviour of activated sludge, and expressed in settling velocity models (Bürger, 2000; Kinnear, 2002; De Clercq et al., 2008). The proposed calibration methods for these settling models, however, require non-destructive monitoring of dynamic settling profiles during batch experiments, for example through radiotracer tests (De Clercq et al., 2005), which are complex to conduct in practice. Therefore, the application of these models is limited to a few cases of 1-D SST modelling (De Clercq et al., 2008; Bürger et al., 2011). Most of the CFD studies consider only the hindered (and flocculent) settling regimes using the empirical formulation of Takács et al. ( 1991). To encourage a broader application of compression settling models by practitioners for the numerical modelling of SSTs, a simple but robust experimental methodology is needed.

## 1.2 Aims of the thesis

This thesis stems from the need to develop more effective numerical tools to predict and mitigate the impact of high hydraulic loadings on the performance of SSTs. The development of model-based decision support tools can then be used to estimate the hydraulic capacity of SSTs and decrease the amount of sewage by-passing under wet-weather conditions.

The overall aim of this thesis is to direct the current WWTP modelling practice towards the application of more advanced second-order 1-D SST models; firstly, by illustrating the significance of selecting the type of 1-D SST model for WWTP modelling under ideal and non-ideal boundary conditions; secondly, by developing experimental and numerical tools for the identification and calibration of more mechanistic second-order 1-D SST models.

This thesis firstly assesses the sensitivity of WWTP model performance to the selection of 1-D SST models with first-order and second-order mathematical structures by means of GSA (**Paper I**). The aim is to illustrate the limitations in the calibration of the first-order SST models over the second-order models for dynamic WWTP simulations.

Following the GSA studies of 1-D SST models, the thesis further aims to supplement the recently published protocol by the International Water Association (IWA) on good modelling practice (GMP) for activated sludge systems (Rieger et al., 2012) with practical findings on the calibration of 1-D SST models (**Paper II**). It is investigated whether the imposed ideal and non-ideal flow (dry- and rain-weather) and settling (good settling or bulking) boundary conditions have an impact on the identification of optimum parameter subset for the calibration of WWTP models, including the SST model parameters.

A significant part of the thesis is dedicated to CFD model development (covered in **Paper III**). The focus is on the optimization of the settling and rheology sub-models using laboratory batch experiments. A novel, simple settling experimental set-up is developed to evaluate the state-of-the-art settling velocity models, which results in the development of a new improved settling velocity model. For calibration, a Bayesian optimization method is used. A 2-D axisymmetric CFD model of a circular SST containing the new settling velocity and rheological model is validated with full-scale measurements.

The validated CFD model with the optimized rheological and settling velocity model is employed in the last study (**Paper IV**) to model the influence of filamentous bulking. This study uses long-term historical data from the rheological and settling measurements, as well as a fluorescent in-situ hybridisation (FISH) analysis performed biweekly for four months by Wágner et al. (D.S. Wágner et al., Impact of filamentous bacteria on the settling and rheology of activated sludge, manuscript in preparation, 2014). CFD simulation scenarios are performed taking into account the impact of filamentous bacteria on the rheology and settling parameters.

In summary, this thesis employs experimental, statistical and numerical modelling tools (Fig. 1.1) to bridge the gap between the development and application of more advanced second-order 1-D SSTs for dynamic WWTP simulations.

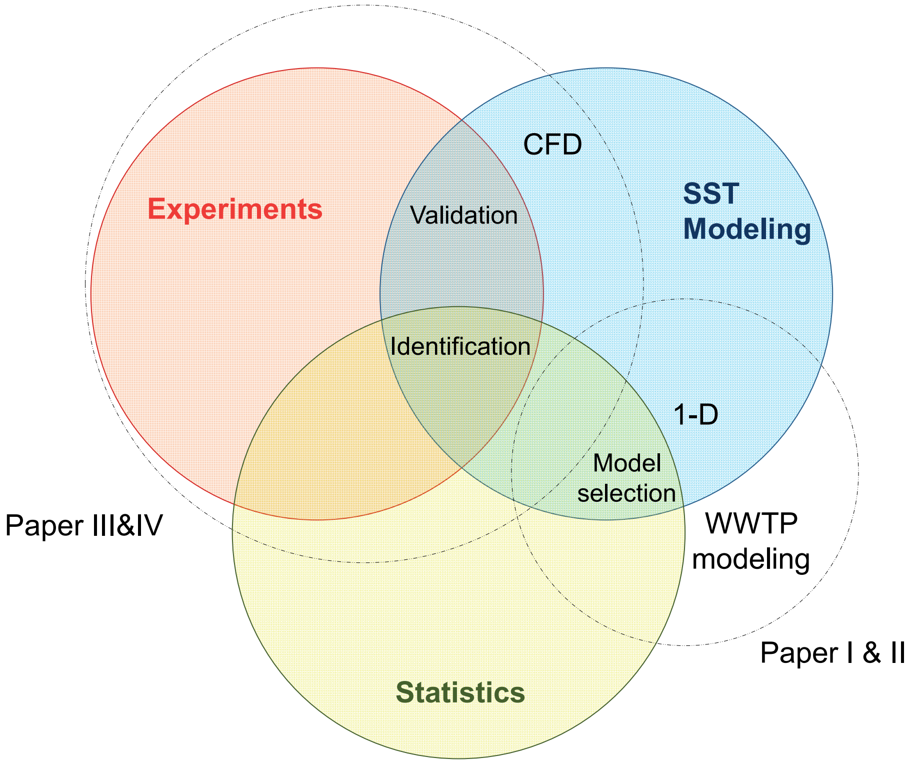


**Figure 1.1** An overview of the experimental (red), statistical (yellow) and modelling (blue) methods applied in this PhD thesis through four journal papers (Paper I, II, III & IV – Appendices of this thesis)

# 2 Description of secondary settling tanks

## 2.1 Function of SSTs

Activated sludge systems are the most common biological wastewater treatment solutions around the world. Figure 2.1 shows the layout of a conventional activated sludge unit, consisting of bioreactors (Fig. 2.1a) connected to secondary settling tanks, SSTs (Fig. 2.1b). In bioreactors, microorganisms suspended as flocs (activated sludge) grow on organic and inorganic constituents (pollutants) in wastewater, and they are separated from the treated water in the SSTs by means of gravity sedimentation. A certain high concentration of biomass is recycled from the bottom of the SSTs to the bioreactors to maintain a desired biomass concentration for efficient conversion of the organic matter in the bioreactors. In fact, SSTs fulfil a triple role in the activated sludge units, acting as a clarifier, a sludge thickener, and during high loading events, as a sludge storage tank.

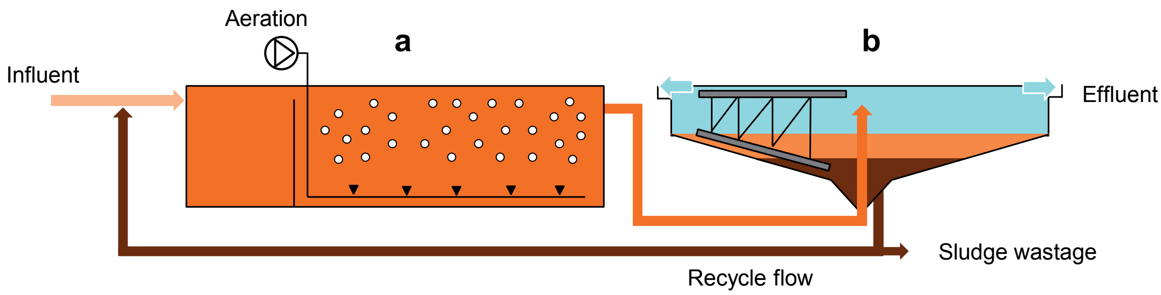


**Figure 2.1** The layout of a conventional activated sludge system including bioreactors (**a**) and secondary settling tanks, SSTs (**b**). The thickened sludge is shown with a darker colour in the SST.

## 2.2 Types of SSTs

The most common types of SST configurations are circular and rectangular. Even though both types perform with the same efficiency if they are well designed, circular SSTs are more common due to lower construction and operational cost. In SSTs with flat bottom, the thickened sludge is removed directly from the bottom by suction pumps. The conical shaped SSTs are equipped with a revolving scraper to transport the sludge from the settled points to the hopper (Fig. 2.2).

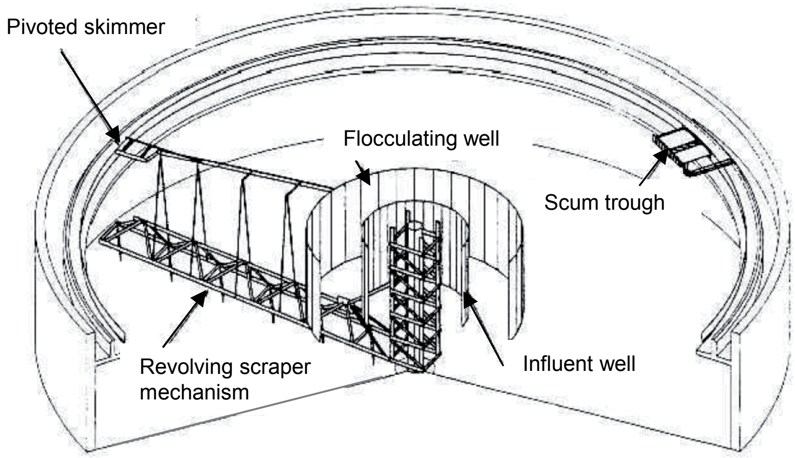


**Figure 2.2** Design of a circular secondary settling tank (SST) with conical shape and equipped with scraper for sludge removal (Ekama et al., 1997).

## 2.3 Performance of SSTs

The thickening and clarification efficiency of an SST is influenced by the activated sludge characteristics and hydrodynamics in the tank (Nopens et al., 2005). In the present thesis, the SSTs are considered non-reactive, i.e. no biological process such as denitrification is assumed to occur in the SSTs. The reader can refer to the study of Gernaey et al. (2006) for the impact of reactive settlers on WWTP simulations.

Even though the settling and flocculation characteristics of sludge originate from biological processes (Wilén et al., 2008, 2010), they have interactive relation with the hydrodynamics in the tank. The fluctuation and floc breakage of sludge depends on the level of turbulence in the sludge transported from the reactors to the SSTs. Fluctuation enhances the settling of sludge by increasing the mass of flocs and thus decreasing the concentration of dispersed suspended solids. The impact of flocculation on the SST performance is not covered in this thesis, and the reader can refer to the PhD thesis of Nopens (2005) for further information on this topic.

The settleability of activated sludge can influence the adopted recycle flow rate and, moreover, limit the maximum permissible flow rate entering the system. These criteria are referred to as the Solids Capacity Criteria (Ekama et al., 1997). Poor settling of activated sludge as a result of excessive filamentous bacteria growth, and occurring under specific operational or seasonal conditions in bioreactors, can hinder the effective operation of SSTs (Martins et al., 2004). The SSTs feature complicated hydrodynamics due to density stratification, which can significantly disturb the sludge distribution in the tank and impact the sludge concentration in the effluent and recycle flow. A malfunctioning SST with a poor quality effluent in terms of suspended solids and insufficiently thickened sludge for recycle to the reactors, impacts the sludge retention time (SRT) in the system, thus potentially deteriorating the biokinetic processes.

## 2.4 Hydrodynamics of SSTs

The first experimental study by Anderson (1945) showed that the flow field in SSTs is far from uniform. The sludge mixture entering the tank is heavier than the ambient water. Therefore, it plunges like a waterfall to the bottom of the tank and creates a horizontal density current with high velocity in the vicinity of sludge blanket. The density current, consequently, generates a counter current to the upper part of the tank, which can have a multiple layer structure in the flow field. Ideally, the layered structure can help with the efficiency of the SSTs by increasing the hydraulic retention time of the solids. However, a strong density current due to very high inflow rates to the plant can disturb the sludge blanket and suspend the settled particles (sludge flocs), and further transport particles to the effluent flow. A schematic of the density current in a circular centre-feed SST with conical bottom is shown in Fig. 2.3.

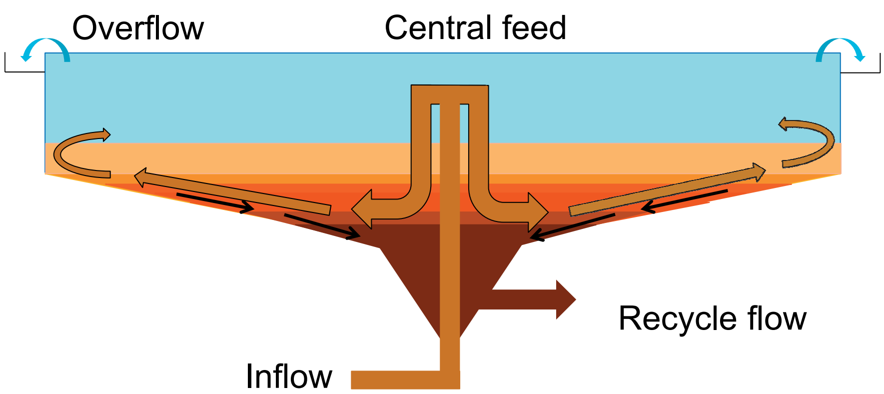


**Figure 2.3** Illustration of induced density current in a circular secondary settling tank with central feed.

Modification of the internal structure of SSTs can reduce the impact of density currents on the solids removal efficiency. An optimized inlet structure with an inlet baffle can reduce the kinetic energy of the inflow as well as the potential energy due to buoyancy (Larsen, 1977; Krebs, 1991; Bretscher et al., 1992; Krebs et al., 1995). The laboratory experiments by Krebs et al.

(1998) showed that increased depth of the tank can help to decrease the deteriorating impact of strong density currents on the effluent quality. Besides, Zhou and McCorquodale (1992) evaluated different designs of SST using numerical tools, and suggested large radiuses for the SSTs with strong density currents.

Overall, considering the utmost importance of SSTs' efficiency for WWTPs performance, a better understanding of the underlying solids mixing and transport processes in SSTs can contribute to the development of numerical tools for model-based decision support purposes.

# 3 Settling of activated sludge

## 3.1 Settling regimes

In a typical activated sludge mixture, particle size varies widely from single bacteria (0.5 to 5 μm) to large flocs (up to 1 mm). Activated sludge flocs consist of a variety of microorganisms, organic and inorganic particles, as well as dead cells, surrounded by extracellular polymeric substances (Wilén et al., 2008). The operational and seasonal variations in activated sludge units influence the microbial population and structure of the growing flocs in bio-reactors, which results in variations in the settling characteristics of sludge.

Most of the theory of the gravitational settling behaviour of activated sludge is based on the work of Coe and Clevenger (1916). They studied the sedimentation phenomena of slurries with mixtures of different particle sizes and recognized four settling classes during batch settling. The diagram in Fig. 3.1 illustrates the four settling classes in relation with the sludge concentration and flocculating properties (Fitch et al., 1958).

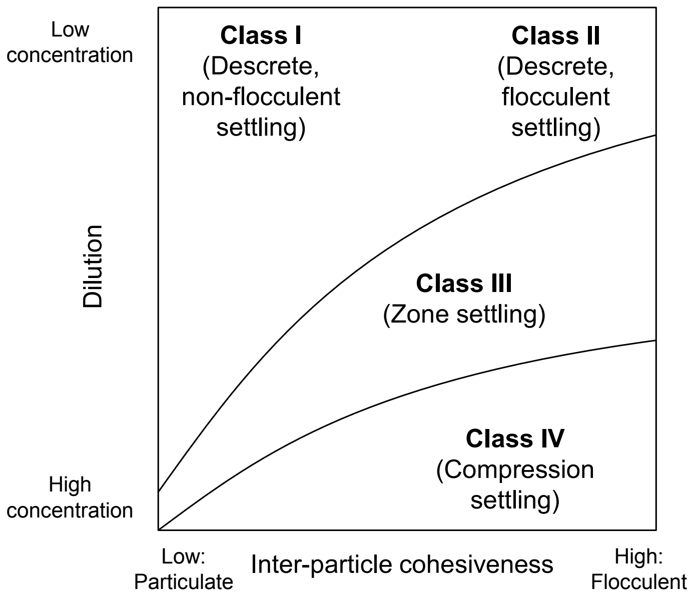


**Figure 3.1** Four classes of activated sludge settling regimes in relation to the sludge concentration (vertical axis) and the flocculating properties (horizontal axis), (Ekama et al., 1997).

In the upper region, at low concentrations, discrete settling (**Class I**) and flocculation settling (**Class II**) occurs. By the increase of concentration in the lower region, the distance between the flocs decreases, and they no longer settle as individuals, resulting in hindered/zone settling (**Class III**). The qualitative argument for the occurrence of zone settling is based on a two phase observation (Probstein, 2003). As the particles settle, an upward movement of water is created which increases the particle drag, and as a result decreases the relative settling velocity of mixture. This phenomena was further analysed theoretically by Kynch (1952) based on the assumption that the particles settle with the velocity that is only a function of local concentration. At the bottom region, where the concentration further increases, the particles, in addition to gravity and drag forces, are exposed to the inter-particle compressive stress and settle slower than in zone settling (**Class IV**).

The settling characteristic of activated sludge is mostly studied by performing batch column settling tests, where the descending liquid/solid interface level (sludge blanket height, SBH) is measured. During the settling test, four different settling regimes are typically identified (Fig. 3.2): (1) lag, (2) hindered/zone, (3) transient, and (4) compression settling (Ekama et al., 1997).

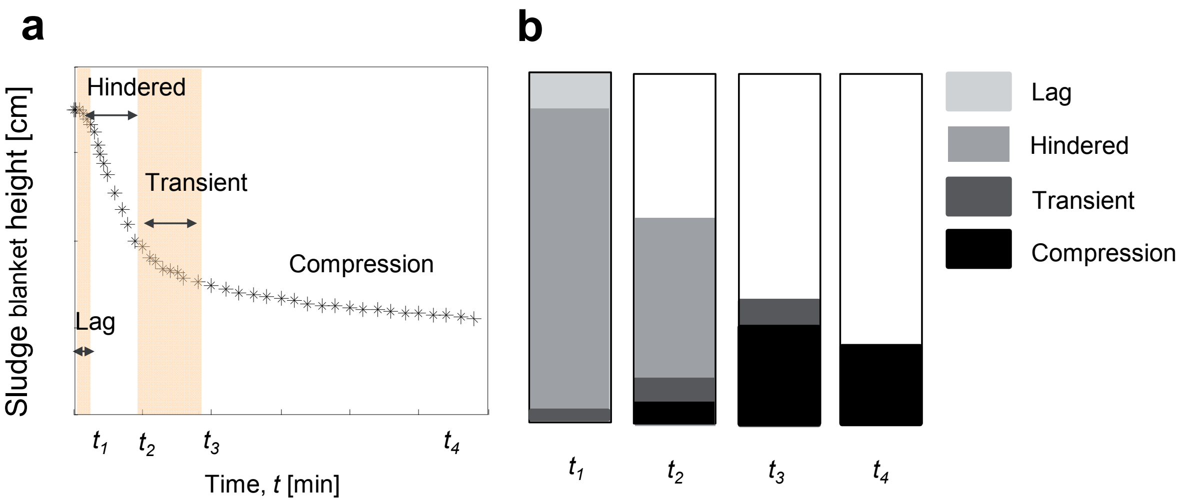


**Figure 3.2** Illustrations of the different settling regimes of activated sludge observed by measuring the sludge blanket height SBH (**a**), during batch column settling tests (**b**).

The lag period observed at the beginning of the SBH measurements results from the dissipation of the kinetic energy introduced with coarse air bubbles to homogenize the sludge in the column before the measurements start. The subsequent constant descending rate of SBH corresponds to the hindered settling velocity of the mixture settling as a whole, with the concentration equal to the initial value. The transition phase between the hindered to compression settling regimes, can be observed in the SBH measurements when the accumulation of sludge at the bottom propagates upwards until it meets the liquid/solid interface.

## 3.2 Filamentous bulking

A common operational problem in SSTs is the poor settling of activated sludge resulting from the excessive growth of filamentous bacteria, which prevents the formation of well-settling sludge (Wanner, 1994). The result is the deterioration of clarification and thickening process and increasing risk of sludge discharge with the effluent. The operational and seasonal variations in activated sludge units, such as dissolved oxygen concentration, nutrient deficiency and substrate limiting conditions, influence the structure of the growing flocs in bioreactors (Comas et al., 2008). However, the exact cause of filamentous bulking can be very diverse (Jenkins et al., 1993), and is not fully understood (Mielczarek et al., 2012). A common approach to identify filamentous bulking is to detect and quantify the content of filamentous bacteria in activated sludge samples by performing quantitative fluorescent *in-situ* hybridisation (qFISH) analysis (Nielsen et al., 2009). Fig. 3.3 illustrates the structure of ideal/good settling flocs (Fig. 3.3a) and filamentous bacteria abundance (Fig. 3.3 b) in activated sludge.

**a** **b**

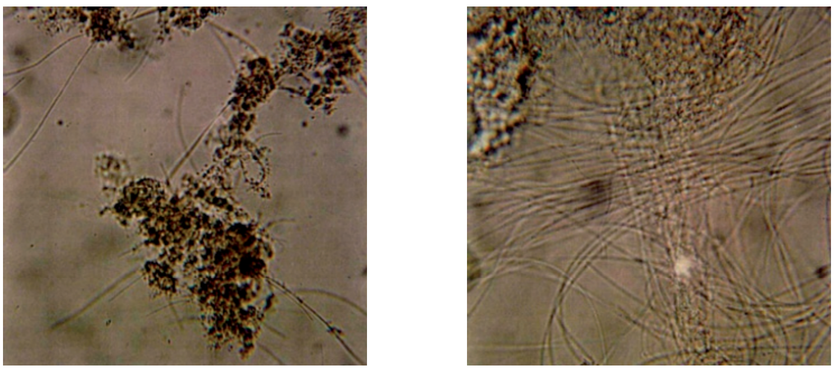

**Figure 3.3** Activated sludge with ideal flocs structure (**a**), and filamentous bacteria abundance (**b**). (Photo taken by B.G. Plósz)

In WWTP modelling, conventionally, the influence of filamentous bulking is directly imposed by modifying the hindered settling parameters in the settling velocity formulation in the SST models (Ekama et al., 1997). Several studies have shown the relation between the morphology of bulking sludge and settling parameters (Grijspeerdt and Verstraete, 1997; Jin et al., 2003; Wilén et al., 2008). However, the question arises whether filamentous bulking can also affect the transient and compression settling—a focal area covered by **Paper IV.**

## 3.3 Settling velocity models

The observations explained in the previous section have led to the development of formulations for settling velocity of activated sludge based on the theoretical and experimental approaches explained in the following.

### 3.3.1 Theoretical approach

A number of mathematical expressions based on theoretical approaches have been proposed to represent the settling velocity of activated sludge. Steinour (1944) presented the settling velocity as a function of the concentration of particles, assuming that the size and density of particles are uniform in Stokes regime (Reynolds number less than 1). Steinour then deduced the settling velocity as a function of void and hydraulic radius. Scott (1966) derived the same result, but with a different hypothesis. His work was based on the Carman-Kozeny equation, an approach which views the thickening process as analogous to the transport of fluid in a non-rigid saturated porous medium, and confirmed that the settling velocity in a column is equal to the average velocity in the porous bed. Cho et al. (1993) formulated a new model based on the Carman-Kozeny equation by adding the slurry viscosity term. The new model showed better correlation compared with the models of Scott and Steinour.

Kinnear (2002) and De Clercq et al. (2008) followed the theory of mixture of classical continuum mechanics (Bustos, 1999; Bürger, 2000), and developed fundamental settling functions to account for compression settling velocity ($v_c$):

$$v_c = v_h\left(1 - \frac{\rho_S}{(\rho_S - \rho_f)gX}\frac{d\sigma}{dX}\frac{dX}{dz}\right) \tag{3.1}$$

where $v_h$ is the hindered settling velocity, $\rho_s$ and $\rho_f$ are sludge and water density, respectively; $g$ denotes the gravity constant; $X$ is the sludge concentration, $z$ is depth; and $\sigma$ is the effective solids stress. The difference between the models developed with this approach is reflected in the formulation of hindered settling and effective solids stress.

### 3.3.2 Empirical approach

Based on the flux theory of Kynch (1952), empirical settling velocity models have been developed to obtain flux curves close to the observations in batch sedimentation experiments (Zeidan et al., 2004). Among the various empirical models suggested over the years, the exponential formulation by Vesilind (1968) was the most widely accepted. This equation is applied to describe only hindered settling, and the parameters can be obtained from a series of batch tests over a concentration range, by measuring the zone settling velocities as the constant descending rate of the liquid/solid interface. Takács et al. (1991) argued that below the hindered settling concentration, settling velocities predicted by Vesilind's equation exceed the actual settling velocity predicted by Li and Ganczarczyk (1987). Therefore, they proposed an extension to Vesilind's settling velocity model to decrease the predicted velocity to realistic values for low concentrations:

$$v_S = \min(v_0 e^{-r_H X(1-fns)} - v_0 e^{-r_P X(1-fns)}, v_{\max}) \tag{3.2}$$

where $v_0$ is the ultimate settling velocity; $r_H$ and $r_P$ are the hindered and low concentration (or flocculent) settling characteristic indices, respectively; $f_{ns}$ is the non-settling fraction; $v_{max}$ is the maximum attainable settling velocity imposed to suppress unrealistically high settling velocity values. $v_{max}$ was not necessary in further applications of the model and has been mostly eliminated from the formulation (Plósz et al., 2007; Takács, 2008). In response to the argument posed that, theoretically speaking, the average settling velocity of particles in the flocculent settling zone is independent of concentration, based on the understanding of discrete particle settling, Patry and Takács (1992) demonstrated that the average settling velocity of flocculent suspensions is correlated to the suspended solids concentration (Takács, 2008).

One of the drawbacks in the application of the hindered settling velocity function (Eq. 3.2) is the time-consuming calibration procedure including a series of batch settling tests (see section 3.4.1). To facilitate this process, a Settlometer (Vanrolleghem et al., 1996, Applitek NV, Belgium) was developed to automatically record batch settling curves. Vanderhasselt and Vanrolleghem (2000) investigated the validity of single batch settling curve (SBSC) methods, indirectly estimating the parameters of settling velocity models compared to the traditional dilution experiments. They encountered identifiability problems associated with the estimated parameters from a SBSC with the settling velocity models of Vesilind (1968), Takács et al. (1991), and Cho et al. (1993), and concluded that the batch experimental setups should be modified to obtain more data points for the high settling rates, e.g. faster detection of sludge blanket height. Vanderhasselt and Vanrolleghem (2000) also suggested continuous column settling tests to better study the hindered and transient settling. Such a setup was used before by Rasmussen and Larsen (1996) in their study on settling velocity under turbulence conditions.

Diluted Sludge Volume Index, DSVI (Stobbe, 1964) is the most commonly measured parameter in WWTPs to quantify the settling characteristics of activated sludge. DSVI is obtained from a simple settling test in a 1 Liter column with a diluted sludge sample (to eliminate the effect of sludge concentration), where the volume of the settled sludge per gram of solids is measured after 30 minutes. White (1975) introduced a more reliable measure of activated sludge settlability, the stirred specific volume index at 3.5 g/l ($SSVI_{3.5}$) defined as the volume of a unit mass of sludge settled for 30 minutes in a settling column equipped with a gentle stirring device. Even though there is no evidence of a mechanistic relation between DSVI or $SSVI_{3.5}$ and the hindered settling parameters ($r_H$, $v_0$) in the literature, there have been attempts to establish empirical correlations for practical reasons (Ekama et al., 1997):

$$v_0 = \alpha \exp(-\beta \times SSVI_{3.5}) \tag{3.3}$$

$$r_H = \kappa + \lambda \times SSVI_{3.5} \tag{3.4}$$

where $\alpha$, $\beta$, $\kappa$, and $\lambda$ are the constants.

In general, the settling velocity models are incorporated in SST models as well as in state-point analysis for the purpose of SST design or operation (Ekama et al., 1997). However, the focus of this thesis is on the numerical models that can describe the dynamics of SSTs (see section 4).

## 3.4 Calibration of settling velocity models

The accuracy of the settling velocity models in section 3.3.depends on the quality of their calibration to experimental data.

### 3.4.1 Calibration of hindered settling velocity model

The estimation of hindered settling parameters ($r_H$ and $v_0$ in Eq. 3.2) is straight forward. A series of batch settling tests with different initial sludge concentrations are performed, where the SBH is measured for 30 minutes (Fig. 3.4a). The hindered settling velocity of each settling curve is obtained as the constant descending rate of SBH with time (e.g. solid line in Fig. 3.4a). The hindered settling velocities are then correlated to the initial sludge concentrations with an exponential relation (Fig. 3.4b).

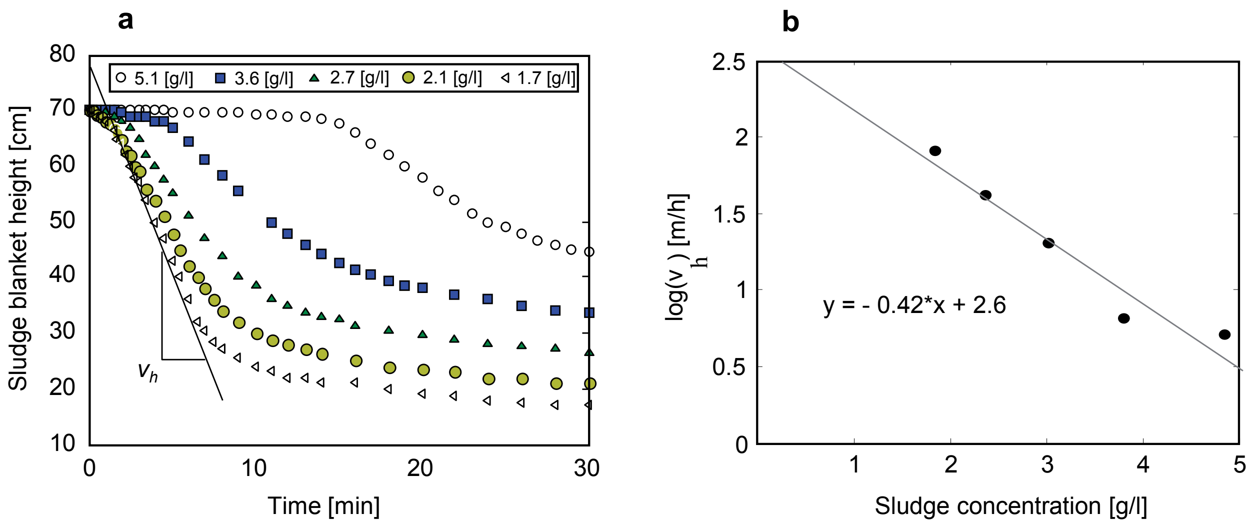


**Figure 3.4** Estimation of hindered settling parameters $r_H$ and $v_0$ (Eq. 3.2) from the SBH measurements (**a**), by correlating the hindered settling velocity, $v_h$, to the initial sludge concentrations (**b**).

## 3.4.2 Calibration of compression settling velocity model

To calibrate more advanced, mechanistic-based settling velocity models such as the compression settling velocity model in Eq. 3.1, more measurements are required. As mentioned in section 3.2, only fitting the settling velocity function to the SBH curve, which partly incorporates the effect of transient, and compression settling regimes, creates identifiablility problems for the settling velocity model parameters. De Clercq et al. (2005b) performed a detailed monitoring of sludge profile dynamics during batch settling experiments using radiotracer tests. They could then calibrate the compression settling velocity to the measured profiles. This calibration procedure is, however, not simple in practice. The question arises whether a simple batch experiment with additional measurements to the SBH measurements can provide sufficient data to identify parameters for the calibration of compression settling velocity models. To answer to this question, in **Paper III** of this thesis an experimental methodology using a simple batch experiment was developed, in which, in addition to SBH measurements, the sludge concentration at the bottom was measured (Fig. 3.5, plotted marks). The compression settling velocity model was then implemented in a 1-D model of the settling column (see section 4.1) and fitted to both measurement curves using the recently developed Differential Evolution Adaptive Metropolis (DREAM$_{(ZS)}$) algorithm (Vrugt et al., 2009; Laloy and Vrugt, 2012).

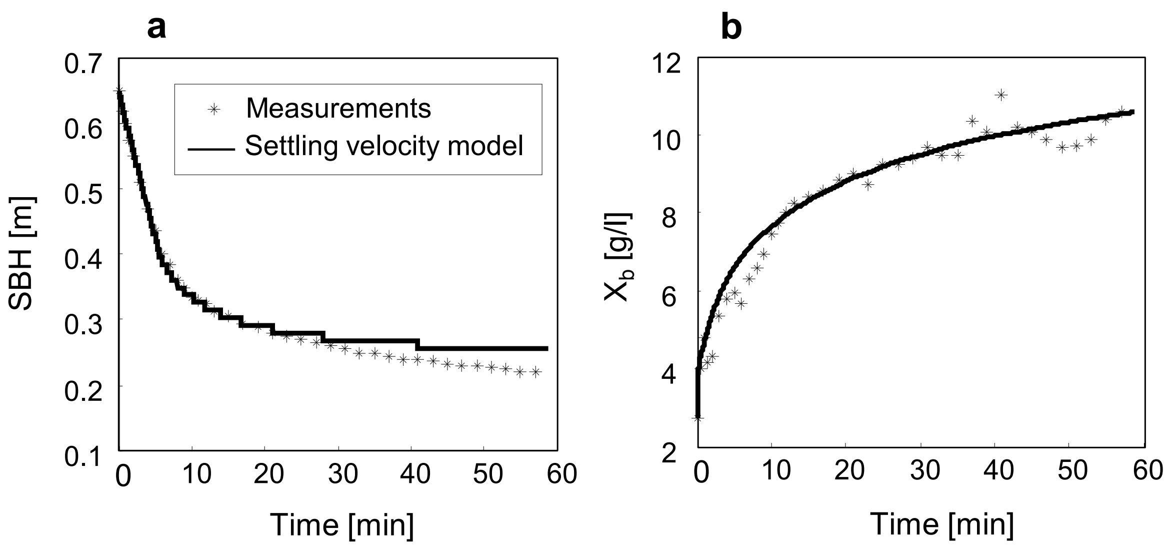


**Figure 3.5** A new proposed experimental methodology in this thesis (**Paper III**) to calibrate the compression settling velocity model by fitting the model to the measurements of sludge blanket height, SBH (**a**), and sludge concentration at the bottom (**b**) using DREAM$_{(ZS)}$ optimization algorithm.

The DREAM$_{(ZS)}$ method is developed in the Bayesian framework. The Bayesian theorem, named after Thomas Bayes (c. 1702–61), is based on the consideration that the observations ($x$) and model parameters ($\theta$) are random quantities (in contrast to the classical approach that considers parameters as fixed unknown values). Knowing the parameters probability $P(\theta)$, as well as the likelihood function of $\theta$ for given $x$ (i.e. the probability of predicting $x$, with the model parameters $\theta$), $P(x|\theta)$, the distribution of $\theta$ conditional on $x$ is then determined as:

$$P(\theta|x) = \frac{P(\theta)P(x|\theta)}{\int P(\theta)P(x|\theta)d\theta} \tag{3.5}$$

Where $P(\theta|x)$ is called the posterior distribution of $\theta$, which is used to estimate the probability interval of model predictions.

The DREAM$_{(ZS)}$ method uses the Monte Carlo Markov Chain (MCMC) algorithm to provide random walks from the current to a new position in the parameter space until the solution converges to an stationary posterior distribution within an acceptable error range. The MCMC algorithm is optimized in the DREAM$_{(ZS)}$ method using a self-adaptive randomised subspace sampling method, which significantly reduces the number of steps required to achieve convergence. The DREAm$_{(ZS)}$ optimization method has been used in many environmental fields such as hydrological modelling (e.g. Laloy and Vrugt, 2012), and crops modelling (e.g. Dumont et al., 2014).

# 4 Modelling of secondary settling tanks

Mathematical models of a system are developed to quantify the future or hypothetical behaviour of a system. They are described as ‘machines’ that transform the input data to the output data through defined mathematical relations (Dochain and Vanrolleghem, 2001). In the classification of the mathematical model, the state-space models consist of a set of input, output, and state variables (e.g. concentration, velocity, etc.) related by a set of algebraic, ordinary, and/or partial-differential equations formulated based on the transport processes and conservation laws (Gujer, 2008).

The mathematical structure of an SST model is built based on the simplifications made in terms of space dimension (zero-, 1-D, 2-D, 2-D axisymmetric, 3-D), and the description of the transport processes (advection, gravity settling, dispersion, flocculation, turbulence, etc.). The present thesis focuses on 1-D models and 2-D axisymmetric models.

## 4.1 One-dimensional SST models

1-D SST models are predominantly used in conjunction with the Activated sludge Model (ASM) family (Henze et al., 2000) for the dynamic modelling of activated sludge units.

The conservation and transportation of mass in the SST can be described mathematically in 1-D. There are two mathematical approaches in formulating the mass balance, namely the widely used first-order and the recently developed second-order approach.

### 4.1.1 First-order approach

The first-order mathematical approach uses hyperbolic (first-order) partial differential equations (PDEs) based on the flux theory of Kynch (1952), which assumes that settling velocity depends only on the local sludge concentration:

$$\frac{\partial X}{\partial t}+\frac{\partial F(X)}{\partial z}=0 \tag{4.1}$$

where $X$ is the sludge concentration, $t$ denotes time, and $F$ is the solids flux at depth $z$ of the settler. The flux accounts for the settling flux of particles and bulk convection flux:

$$F(z,t) = vX - v_s X \tag{4.2}$$

where $v_s$ is the settling velocity, and $v$ is the bulk downward flux due to the recycle flow below the feed position and the bulk upward flux due to overflow above the feed position. $v$ is hence simply calculated as the ratio of recycle or over flow rate to the settlers surface area, depending on the relative position to the feeding point.

The solids transport equation (4.1) is solved numerically by discretizing it to several horizontal layers along the depth of the settler, with the assumption that the sludge concentration is uniform in each layer. However, the hyperbolic nature of the equation creates shock waves along the depth, which results in reverse concentration gradients in some layers, i.e. the concentration of the layers above becomes higher than the one below. To obtain a smooth profile concentration using the hyperbolic 1-D model, Takács et al. (1991) used the limiting flux conditions by Stenstrom (1976) to avoid the creation of shock waves in the solution—an *ad hoc* assumption with no physical meaning (De Clercq, 2006). Additionally, they limited the number of layers to 10 to introduce a high numerical dispersion, and thus further improve the numerical behaviour of the model. Numerical dispersion is the result of approximating the solution of partial differential equations by difference equations in the finite elements of the discretized time and space domain. For example, the forward finite difference approximation of the $X$ gradient in the $i$th layer is:

$$\frac{\partial X}{\partial z} \approx \frac{X_{i+1} - X_i}{\Delta z} \tag{4.3}$$

The coarser the discretization of the space domain (i.e. the larger $\Delta z$), the larger the error introduced to the solution. In case of first-order models, this error favours the numerical behaviour of the hyperbolic equation. However, as stated by Plósz et al. (2011), the drawback of this approach is the lack of control over the introduced numerical dispersion, which limits the validity of model prediction into narrow flow boundary conditions. Moreover, this approach considers the number of layers as a model parameter, thus violaing the consistant modeling methodology proposed by Bürger et al. (2011). In the framework of first-order models, it is impossible to obtain a realistic mesh-independent concentration profile, as the restriction on the flux disappears if the number of grids converges to infinity (Watts et al., 1996; Verdickt et al., 2006; Plósz et al., 2007, 2011).

### 4.1.2 Second-order approach

The parabolic (second-order) modelling approach has been developed to overcome the drawbacks of the first-order models by including an explicit dispersion term in the mass balance equation (Watts et al., 1996; Diehl and Jeppsson, 1998; Joannis et al., 1999; Lee et al., 1999; Kinnear, 2002; De Clercq et al., 2003, 2008; Plósz et al., 2007; Bürger et al., 2011):

$$\frac{\partial X}{\partial t} + \frac{\partial F(X)}{\partial z} = \frac{\partial}{\partial z}\left(D\frac{\partial X}{\partial z}\right) \tag{4.4}$$

where $D$ is the dispersion coefficient. The dispersion term in Eq. 4.4 is imposed as an entropy condition to obtain physically meaningful and unique solutions (Bürger et al., 2011). This term lumps all of the hydraulic features of the SST, e.g. turbulence, compression, density current and sludge removal effects (Ekama et al., 1997). In the second-order model by Plósz et al. (2007), a dynamic feed layer (Dupont and Dahl, 1995), with depth limitation and a feed-flow dependent convection reduction factor, was introduced to approximate the impact of horizontal density currents in 1-D. The latter factor was applied to reduce the 3-D downward conveyance velocity of sludge to the withdrawal point in the real system to a vertical movement in 1-D:

$$\frac{\partial X}{\partial t} + \frac{\partial(\eta v X - v_S X)}{\partial z} - \frac{\partial}{\partial z}\left(D_C\frac{\partial X}{\partial z}\right) = v_F X_F \delta(z) \tag{4.5}$$

where $\eta$ is the convective reduction factor; $D_C$ is the flow dependent dispersion coefficient; $v_F$ and $X_F$ are the velocity and sludge concentration of the inflow, respectively; and $\delta$ is the Dirac delta distribution. The novelty of their work lies in their use of a 2-D axisymmetric CFD model of a flat-bottom circular SST to generate data in a range of feed flow rates, and thus calibrate the dispersion coefficient and the reduction factor of the 1-D model. They identified correlations describing the dispersion dependent on the overflow rate, and the reduction factor dependent on the feed flow rate. For detailed formulation of $\eta$ and $D_C$, the reader is referred to the work of Plósz et al. (2007). Their approach motivated this thesis to develop a CFD model for the future research on the identification of more mechanistic flow (and design) dependent hydraulic terms in second-order 1-D SST models.

The numerical solution of Eq. 4.5 is performed by discretizing it to a finite number of layers (Fig. 4.1). In contrast to the first-order approach, the number of layers is not limited, and in fact, it should be sufficiently increased to achieve a mesh independent solution, while keeping in mind the computational constrains for 1-D models. The optimum number of layers is between 60 and 100, depending on the structure of the dispersion term, accounting for compression settling velocity or for solids dispersion (De Clercq et al., 2008; Bürger et al., 2012), or a flow dependent dispersion (Plósz et al., 2007).

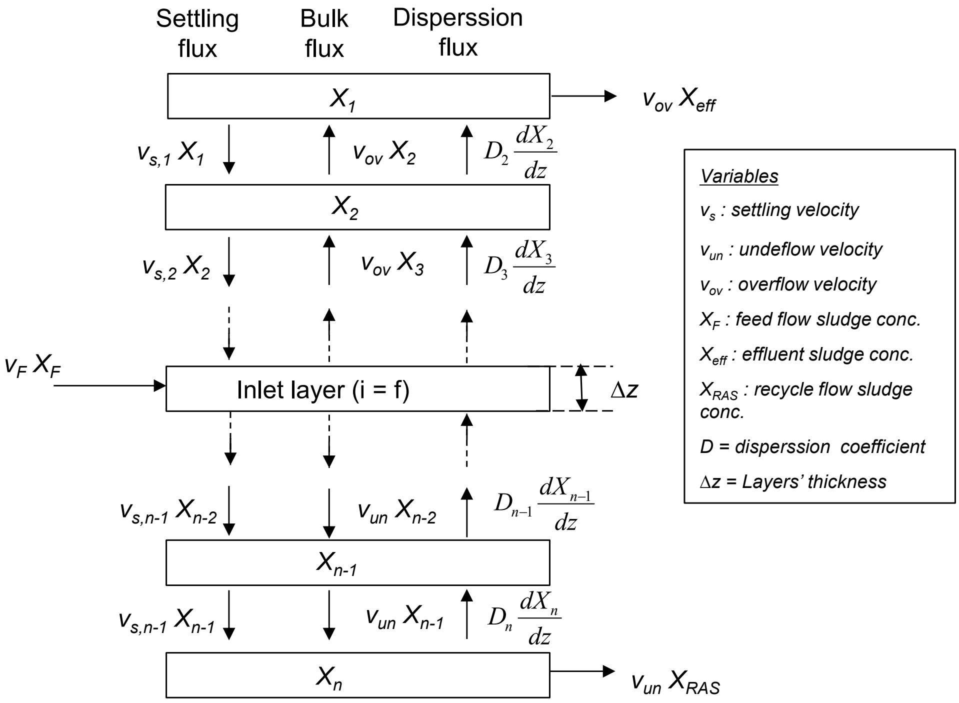


**Figure 4.1** Discretization of the second-order mass balance equation of an SST to a finite number of horizontal layers.

The numerical approximations of the fluxes in equation 4.4 are not linear (e.g. the settling flux) and they further contain space discontinuities (e.g. the bulk convective flux, *F*). In order to estimate accurate and smooth concentration profiles, the numerical fluxes are treated by applying numerical algorithms that impose an entropy condition, e.g. an Engquist-Osher (Engquist and Stanley, 1981) or a Godunov (Godunov, 1959) type scheme. The Engquist-Osher method is used by Bürger and Karlsen, (2001) and De Clercq et al. (2008, 2005a), and is reported to be more accurate than the Godunov method (Bürger et al., 2011). The Godunov method, on the other hand, is easier to implement and requires less computation, and is therefore more widely used (Diehl et al., 1990; Jeppsson and Diehl, 1996; Bürger et al., 2005, 2011, 2013; Plósz et al., 2007):

$$F(X_i,t)=\begin{cases}\min(F(X_i,t),F(X_{i+1},t)) & if\ X_i \geq X_{i+1}\\ \max(F(X_i,t),F(X_{i+1},t)) & if\ X_i < X_{i+1}\end{cases} \tag{4.6}$$

where $X_i$ is the sludge concentration of the $i^{\text{th}}$ layer.

## 4.2 Computational fluid dynamics (CFD) models

To predict the internal flow field and solids distribution in the SSTs, complex computational fluid dynamics (CFD) models have been developed. CFD models are based on solving the non-linear hydrodynamic PDEs of mass and momentum conservation—known as Navier-Stokes equations— and turbulence equations using numerical algorithms (Ferziger and Perić, 1996; White, 2006). The CFD models, in combination with suitable boundary conditions, can approximate the velocity vectors and turbulent mixing coefficients with very good accuracy.

As mentioned earlier, validated CFD models are potential tools for the development of more mechanistic second-order 1-D SST models. By continuous advancements in the performance of computers and servers, and the decreasing costs of hardware, the use of CFD models have become more popular in the study of the behaviour of systems under different operational scenarios. CFDs can replace the expensive and time-consuming experimental studies, which may not be feasible to perform under extreme conditions. Additionally, CFD models can provide more detailed information on the flow field in the system, which cannot be measured.

Since the first CFD model of a rectangular SST, developed by Larsen (1977), research has sought to improve the prediction of the CFD models by optimizing their mathematical structure in terms of turbulence, and buoyant flow modelling, and in some cases, the settling velocity function and the rheology sub-model (Imam et al., 1983; Adams and Rodi, 1990; Lyn et al., 1992; Zhou and McCorquodale, 1992b; Deininger et al., 1998; Lakehal et al., 1999; De Clercq, 2003; Weiss et al., 2007).

### 4.2.1 Flow field and solids transport

Different approaches exist to modelling the flow field and solids transport in a density driven turbulent flow. In the Eulerian two-phase approach, the solids phase is considered as a continuum, and the momentum and continuity equation is written for both the solid and the liquid phase (Elghobashi, 1994; Rasmussen, 1997). In practice, this approach is very computationally demanding and, generally, models with one momentum equation have been used instead. In the single phase modelling approach, the two-phase mixture is treated as a single fluid phase with variable density, and the buoyant effects are included by modifications in momentum and turbulence equations (e.g. Adams and Rodi, 1990). In order to predict the distribution of the dispersed phase within the mixture, a convection diffusion equation from the continuity equation of the dispersed phase is coupled with the momentum equation. The models developed based on this approach are called diffusion or *drift-flux* models.

Another approach was applied by Brennan (2001), by averaging the Eulerian two-phase flow hydrodynamic equations based on the mixture centre of mass (Ishii, 1975). To describe the relative motion of phases, the following kinematic constitutive equation is applied. For the phase fraction

$$\alpha_1 + \alpha_2 = 1 \tag{4.7}$$

and the mixture density

$$\rho_m = \alpha_1 \rho_1 + \alpha_2 \rho_2 \tag{4.8}$$

the centre of mass mixture velocity is defined as

$$v_m = \frac{\alpha_1 \rho_1 v_1 + \alpha_2 \rho_2 v_2}{\rho_m} \tag{4.9}$$

The velocity of each phase relative to the centre of mass, and the phase velocity $v_k$ ($k$ = 1 or 2) is derived as

$$v_{km} = v_k - v_m \tag{4.10}$$

The velocity relations of the two phase flow are illustrated in Fig.4.3.

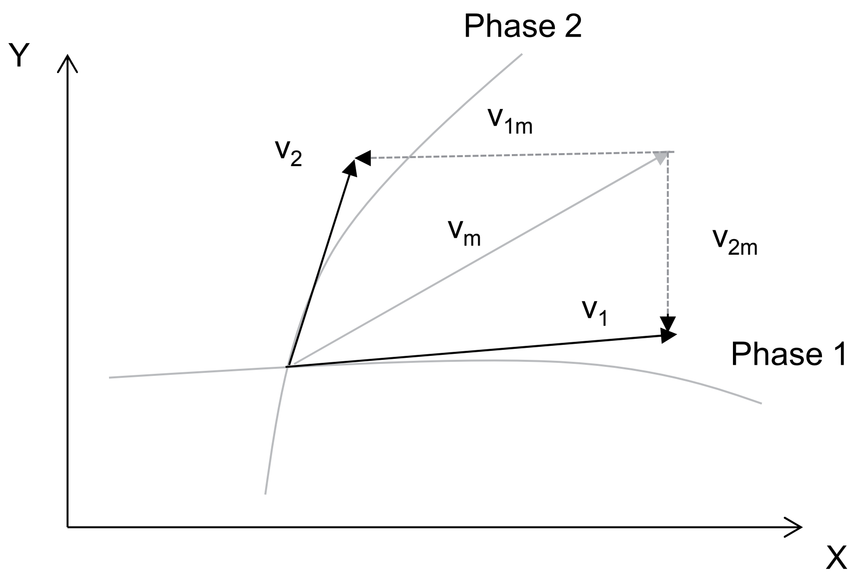


**Figure 4.3** The relations between velocity vectors (→) of the two phase stream lines (─) in the averaged Eulerian two-phase approach (Brennan, 2001).

Consequently, the relation between the relative velocity of the fluid phase and the drift velocity of the solids phase (the settling velocity, see section 3.2) can be obtained as

$$v_{2m} = \frac{\alpha_1 \rho_1}{\alpha_2 \rho_m} v_s \tag{4.11}$$

The model was then formulated in terms of the solids fraction and the settling velocity, where the mixture continuity equation is

$$\frac{\partial \rho_m}{\partial t} + \nabla.(\rho_m v_m) = 0 \tag{4.12}$$

the mixture momentum equation is

$$\frac{\partial \rho_m v_m}{\partial t} + \nabla.(\rho_m v_m v_m) = -\nabla.P_m + \nabla.\left[\tau + \tau^t\right] - \nabla.\left(\frac{\alpha_d}{1-\alpha_d}\frac{\rho_d \rho_c}{\rho_m} v_s v_s\right) + \rho_m g \tag{4.13}$$

and the drift equation for the prediction of solids distribution is

$$\frac{\partial \alpha_d}{\partial t} + \nabla.(\alpha_d v_m) = -\nabla.\left(\frac{\alpha_d \rho_c}{\rho_m} v_s\right) + \nabla.\Gamma\nabla\alpha_d \tag{4.14}$$

where $P_m$, $\rho_m$ and $v_m$ are the average pressure, density, and velocity of mixture, respectively; $\partial$ is the partial derivative; $\nabla$ is the vector differential operator *del*; $t$ denotes time; $\tau$ and $\tau^t$ are the molecular and turbulent shear stress tensors, respectively; $\alpha_d$ is the volume fraction of the dispersed phase; $\rho_c$ and $\rho_d$ are the density of the continuous and dispersed phase, respectively; $v_s$ is the settling velocity of dispersed phase; $g$ is the gravity constant; $\Gamma$ is the turbulent diffusion coefficient, which is made equal to the turbulent viscosity, in direct analogy to the mass and momentum transport.

### 4.2.2 Turbulence

"Turbulence is a three dimensional time-dependent motion in which vortex stretching causes velocity flocculation to spread to all wavelengths between a minimum, determined by viscous forces, and a maximum, determined by the boundary conditions of the flow."(Bretscher et al., 1992)

Turbulence in SSTs is mostly created by the influent with high kinetic energy mixing with the flow in the tank. Due to the complex characteristics of turbulent flows, it is very difficult to predict them theoretically. In addition, due to the small elements in turbulence flow, the numerical solutions for the Navier-Stokes turbulence equations are very computational demanding. To address these complexities, semi-empirical equations based on averaging of the conservation equations and empirical relations are developed (Rodi, 1993). Most of the semi-empirical turbulence models are based on Boussinesq's eddy viscosity concept, which assumes that the turbulence stresses are proportional to the mean velocity gradients in analogy to viscous stresses in laminar flows (Stokes' viscosity law). Turbulence viscosity, in contrast to the molecular viscosity, is not a fluid property and is only the function of the turbulent state of the flow. Among a number of semi-empirical two-equation turbulence models (Menter, 1994), the most commonly used model to determine the distribution of the eddy viscosity over the flow field, is the *k*-*ε* model, which relates the eddy viscosity to the turbulent kinetic energy *k* and the turbulent energy dissipation rate *ε* through the following empirical equation:

$$\mu_t = \rho_m C_\mu \frac{k^2}{\varepsilon} \tag{4.15}$$

The buoyancy modified transport equations for *k* and *ε*, which account for density stratification (Dahl, 1993; Rodi, 1993) are given as the following form:

$$\frac{\partial \rho_m k}{\partial t} + \nabla.(\rho_m v k) = \nabla.\left[\frac{\mu_t}{\sigma_t}\nabla k\right] + P_k + G_k - \rho_m \varepsilon \tag{4.16}$$

$$\frac{\partial \rho_m \varepsilon}{\partial t} + \nabla.(\rho_m v \varepsilon) = \nabla.\left[\frac{\mu_t}{\sigma_t}\nabla \varepsilon\right] + C_{1,\varepsilon}\rho_m \frac{\varepsilon}{k}(P_k + G_k - C_{3\varepsilon}G_k) - C_{2,\varepsilon}\rho_m \frac{\varepsilon^2}{k} \tag{4.17}$$

where $P_k$ is the generation of turbulence kinetics energy due to mean velocity gradients:

$$P_k = \mu_t \left(u'^2 + v'^2 + w'^2\right) \tag{4.18}$$

and $G_k$ corresponds the generation of turbulence kinetics energy due to buoyancy:

$$G_k = -g \frac{\mu_t}{\rho_m \sigma_t} \frac{\partial \rho_m}{\partial z} \tag{4.19}$$

The constants in the above equations are: $C_\mu = 0.09$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_{3\varepsilon} = 0.85$, $\sigma_t = 1.0$, $\sigma_\varepsilon = 1.2$ (Brennan, 2001).

### 4.2.3 Rheology

Rheology is the science of the flow phenomena as observed in the viscous characteristics of a specific liquid. Theoretical aspects of rheology include the relation of the flow/deformation behaviour of material and its internal structure. Much of theoretical rheology is concerned with associating external forces and torques with internal stresses and internal strain gradients and velocities. The typically observed rheological behaviours are illustrated in Fig. 4.4. Newtonian fluids like water, show a linear relation between shear rate and shear stress, i.e. they have a constant viscosity independent of the shear rate conditions. Non-Newtonian fluids, on the other hand, possess an internal shear stress, i.e. they have a constant viscosity independent of the shear rate conditions. Non-Newtonian fluids, on the other hand, possess an internal structure, and behave differently under different shear rate conditions. The shear rate dependent viscosity is referred to as *apparent viscosity*.

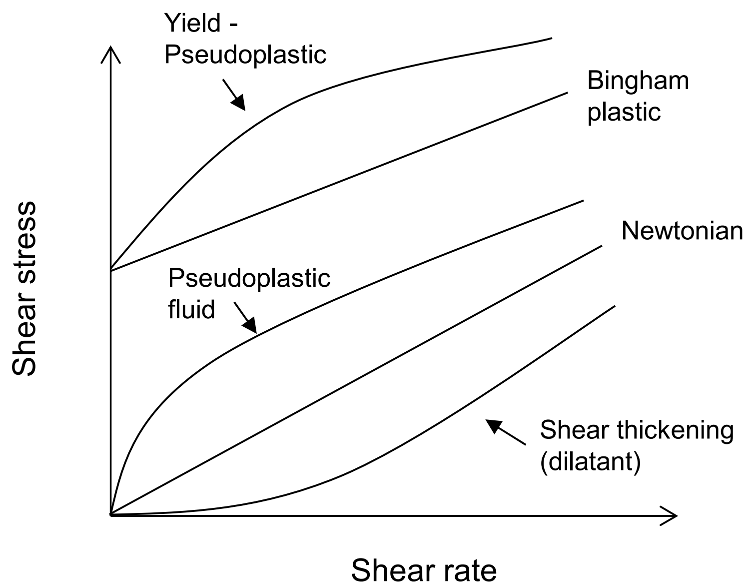


**Figure 4.4** Typical rheological behaviour of fluids (Ratkovich et al., 2013).

Activated sludge is considered to behave as a non-Newtonian fluid (Eshtiaghi et al., 2013; Ratkovich et al., 2013). In CFD modelling of SSTs, due to turbulence damping by stratification in the solids blanket at high sludge concentration low shear rate regions, the eddy viscosity becomes equal to and/or smaller than the sludge viscosity. As a result, to predict the hydrodynamics of the system more accurately, the sludge viscosity needs to be included in the model. Consequently, modelling the flow field in the vicinity of the sludge blanket requires the inclusion of a proper rheological model for sludge viscosity (Ratkovich et al., 2013). In SSTs with conical shape, the sludge rheology is very important for transporting the thickened sludge at the bottom of the tank to the hopper for removal.

There are many empirical formulas in the literature that relate the apparent viscosity of activated sludge to the induced shear rate by convective flow in the system. The three most used ones are listed in Table 4.1. To calibrate these models, rheological measurements are carried out in a rheometer to establish a relationship between the applied external force (shear stress) and the measured internal velocity gradients (shear rates).

**Table 4.1** The three most common rheological models in literature to describe the non-Newtonian behaviour of activated sludge

| Model | Equation | Parameters | Example |
|---|---|---|---|
| Bingham | $\mu = \frac{\tau_0}{\gamma} + \mu_p$ | $\tau_0$ : yield stress [Pa]<br>$\mu_P$ : plastic viscosity [Pa s] | Lakehal et al. (1999) |
| Casson | $\mu = \left(\frac{K_1}{\gamma^{0.5}} + K_2\right)^2$ | $K_1$ : Casson yield stress parameter [$Pa^{0.5}$]<br>$K_2$ : Casson viscosity parameter [$Pa\ s^{0.5}$] | Chhabra and Richardson (2008) |
| Herschel-Bulkley | $\mu = \frac{\tau_0}{\gamma} + K\gamma^{n-1}$ | $\tau_0$ : yield stress [Pa]<br>$K$: consistency index [$Pa\ s^n$]<br>$n$: power law exponent [-] | Craig et al. (2013) |

Combined models such as Casson and Bingham (Weiss et al., 2007) or Herschel-Bulkley and Bingham (Eshtiaghi et al., 2013) are shown to give a good description of the activated sludge rheology up to very high values of shear rates. In CFD modelling, the computational efficiency of continues rheology models is preferable to the combined models with discontinuity at the switching point.

The rheological behaviour of sludge is known to be a function of temperature and sludge concentration (Yang et al., 2009; Novarino et al., 2010). For this reason, mostly empirical correlations have been defined for the different parameters in the rheological models as functions of sludge concentration and temperature (Weiss et al., 2007; Ratkovich et al., 2013).

### 4.2.4 Settling

Settling is a one-dimensional process in nature; therefore, in the CFD models of SSTs, the empirical settling velocity functions calibrated to measurements from batch settling tests (section 3) are used in the continuity equations. The most widely used velocity function in CFD modelling is the double exponential function developed by Takács et al. (1991), Eq. 3.2 (e.g. Lakehal et al., 1999; Weiss et al., 2007; Zhou and McCorquodale, 1992). However, Takács model only describes the hindered and low concentration settling regimes. The mechanistic compression settling models developed based on phenomenological sedimentation-consolidation theory (Bürger et al., 2000) have not been implemented so far in the CFD models—a focal area of this thesis covered in **Paper III**.

### 4.2.5 An open source CFD tool: OpenFOAM

OpenFOAM (Open Field Operation Manipulation) is an open source CFD toolbox with a generic modelling platform for solving differential equations. The libraries in OpenFOAM are written in C++ for the Linux operation system (Jasak et al., 2007). Since this CFD tool is open source, it is possible to customise and extend the functionality of the existing solvers. OpenFOAM has a highly modular code design, where each functional component (e.g. numerical methods, meshing, physical models, etc.) is compiled into its own shared library. The shared libraries are then simply linked together to execute an application. OpenFoam includes also utilities for data analysis and post-processing.

*Implementation of differential equations*

The hydrodynamic partial differential equations are implemented in OpenFOAM in their natural language, i.e. a top-level code which is a direct representation of the equation. For instance, the general momentum equation:

$$\frac{\partial \rho U}{\partial t} + \nabla.\rho UU - \nabla.\mu \nabla U = -\nabla P \tag{4.20}$$

is represented as:

```
(
 fvm::ddt(rho, U)
 + fvm::div(phi, U)
 - fvm::laplacian(mu, U)
 ==
 - fvc::grad(p)
);
```

*Mesh conversion*

It is possible to use the mesh generated by the commercial software packages in OpenFOAM by converting the mesh format with the available utilities. In this thesis, the software STAR-CCM+® CFD software was used to generate the mesh and was converted for use in OpenFOAM using “ccm26ToFoam” utility.

*Visualisation*

The OpenFOAM simulation cases can be visualised using the open source based graphic tool *Paraview*, which uses the Visualisation Toolkit (VTK) and its data processing and rendering engine that can read any data in VTK-format.

# 5 Significance of SST modelling for dynamic WWTP simulations

## 5.1 Application of global sensitivity analysis (GSA)

The significant advancements in the field of 1-D SST modelling described in chapter 4 are still not available for the practitioners and modellers in the field of wastewater treatment engineering. In most of the commercial packages for WWTP simulations, the first-order 1-D SST model by Takács et al. (1991) is widely used for dynamic WWTP simulations. In the Benchmark Simulation Model No.1, BSM1 (Copp et al., 2002; Alex et al., 2008) and Benchmark Simulation Model No.2, BSM2 (Jeppsson et al., 2007; Nopens et al., 2010; Gernaey et al., 2013), the first-order 1–D SST model of Takács et al. (1991) is used with settling parameter values set in a way that settling poses no real problems to the plant performance.

Influence of selecting first-order and second-order 1-D SST sub-models on the overall performance of WWTP simulation models was rigorously investigated by Plósz et al. (2011) using scenario simulations and measured data. They demonstrated the superiority of second-order to first-order 1-D SST models with an example of the models developed by Plósz et al. (2007) and Takács et al. (1991) in predicting SBH and under flow sludge concentration. They also showed that using the popular first-order Takács model, the feasibility of using measured parameters in the settling velocity function is limited, which is in agreement with the statements of Diehl (1996).

To further assess the significance of 1-D SST model selection in WWTP modelling and calibration, it is important to evaluate and compare the sensitivity of WWTP model outputs to uncertainties intrinsic to the first- and second-order 1-D SST model structures and parameters. Uncertainty analysis estimates the limitation of the model for practical applications and can also be a guide to further improve the model structure (Beven, 2008). Sources of uncertainty reported in literature are grouped as: (i) input uncertainty, and (ii) structural uncertainty (McKay et al., 1999; Sin et al., 2009). The input uncertainty is associated to the influent data and the value of model parameters, which refers to incomplete knowledge about the correct values and can be reduced if the values are measureable. Structural uncertainty is due to the simplifications and assumptions made in the mathematical formulation of the model, which can be reduced by improving the model structure. Quantifying the structural uncertainty is uncommon in literature and needs more research (Sin et al., 2009). Therefore, it is mostly assumed that the uncertainty of the model outputs is related to the model inputs and structural uncertainty is implicitly propagated to the parameters uncertainty (Freni and Mannina, 2010).

Global sensitivity analysis (GSA) has previously been used as an effective tool to identify sources of uncertainty in WWTP models associated with model parameters (Mannina et al., 2006; Beven, 2008; Neumann et al., 2009; Sin et al., 2011; Benedetti et al., 2012; Cosenza et al., 2013a; Sweetapple et al., 2013). In GSA studies, the uncertainty and sensitivity analysis are performed in tandem to assign the uncertainty of model output to different sources of uncertainty in model input (Saltelli et al., 2008). Based on the GSA results, one can assess the sensitivity of WWTP model outputs to the model parameters; therefore GSA is also used as an effective tool to identify parameter subsets for optimum calibration of WWTP models (Sin, 2004; Saltelli et al., 2008; Cosenza et al., 2013a).

## 5.2 GSA methods used in the thesis

### 5.2.1 Linear repression of Monte Carlo simulations

The sensitivity analysis method based on linear regression of Monte Carlo simulations (Saltelli et al., 2008), also called the standard regression coefficient (SRC) method, was employed in this thesis. The SRC method is based on the variance-based GSA approach, where the importance of parameters is quantified by estimating their fractional contribution to the total variance in the model output. As long as the SRC method captures a high percentage of the variance in the model outputs using the multivariate linear regression models built, the method provides reliable results and can replace the more advanced but computationally demanding GSA methods such as Extended-FAST or Sobol's sequence methods. Reliability of the SRC method with reference to the Extended-FAST method is demonstrated by Cosenza et al. (2013b). This method involves (i) specifying the parameter uncertainty; (ii) probabilistic based sampling from the parameters space to generate parameter sets followed by a series of Monte Carlo simulations; and finally, (iii) commutating the parameters sensitivity measures based on the variance decomposition of the model outputs (Step 3).

To generate the samples from the probability distributions of the model parameters, the Latin hypercube sampling technique (Helton and Davis, 2003) is mostly applied since it can efficiently cover the parameter space using a low number of samples. The Monte Carlo simulations of the model using the sampled parameter sets results in "spaghetti plots" of model output time-series (Sin et al., 2009). The 90% percentiles in the band of the spaghetti plots of model outputs indicates the extent of total uncertainty in the model outputs derived from the parameters uncertainty. To quantify the fractional contributions of the uncertain parameters to the total variance in the model outputs, a linear regression is performed between the matrix of sampled parameter sets and the vector of scalar model outputs from Monte Carlo simulations, according to:

$$sy_k = b_{0k} + \sum_{i=1}^{m} b_{k,i}.\theta_i + \varepsilon_k \tag{5.1}$$

where $sy_k$ is a vector of scalar values for the $k^{\text{th}}$ model output; $b_k$ is a vector of coefficients; $\theta_{\text{i}}$ is the $i^{\text{th}}$ sampled parameter set of $m$ dimension; and $\varepsilon_k$ is the error vector of the regression model. The dimensionless form of Eq. 5.1 by employing the corresponding means ($\mu_{syk}$, $\mu_\theta$) and standard deviations ($\sigma_{syk}$,

$\sigma_\theta$) of the outputs and the parameters results in the sensitivity measure ($\beta$) of the parameters corresponding to $sy_k$ (Saltelli et al., 2008):

$$\frac{sy_k - \mu_{syk}}{\sigma_{syk}} = \beta_k \frac{\theta - \mu_\theta}{\sigma_\theta} + \varepsilon_k \qquad (5.2)$$

The coefficient of determination ($R^2$) obtained with the multivariate regression method indicates the proportion of the total uncertainty of the model output explained by the linear model. $\beta$ (also called SRC) is a reliable sensitivity index when $R^2 \geq 0.7$ (Sin et al., 2011), meaning that the linear propagation of parameter uncertainty to model outputs is a valid assumption. The fractional contribution of model parameters to the total variance of model outputs can be calculated as the squared value of the sensitivity measures for each parameter ($\beta^2$).

### 5.2.2 Morris screening

The Morris method was applied in one of the studies of this thesis (**Paper I**) to cross-validate the GSA results obtained using the SRC method.

The Morris method relies on repeated computation of a local sensitivity measure, called Elementary Effect (EE), at randomly selected points in the parameter space following an efficient sampling algorithm proposed by Morris (1991). The EEs for each parameter are obtained from the following differentiation of the $k^{th}$ model output ($sy_k$) with respect to the $i^{th}$ parameter ($\theta_i$):

$$EE_{i,k} = \frac{\partial sy_k}{\partial \theta_i} = \frac{sy_k(\theta_1, \theta_2, \theta_i + \Delta, \ldots \theta_M) - sy_k(\theta)}{\Delta} \qquad (5.3)$$

where $\Delta$ is the predetermined perturbation factor of $\theta_i$, $y(\theta)$ is the scalar model output evaluated at a point in the parameter space, while $y(\theta_1, \theta_2, \theta_i+\Delta, \ldots \theta_m)$ represents the scalar model output corresponding to a $\Delta$ change in $\theta_i$. The value of each parameter is assumed to vary across $p$ levels. In this thesis, $\Delta$, $p$, and $r$ values were defined as 2/3, 4 and 15, respectively.

In order to compare the results of Morris screening with the ones from a Monte Carlo procedure, the mean of the distribution of the absolute values of the elementary effects ($\mu^*$) is used. This was proposed by Campolongo et al. (2007) to solve the problem of type II errors (failing to identify a factor with considerable influence on the model; Saltelli, 2006):

$$\mu_i{*} = \frac{1}{r}\sum_{j=1}^{r} \left| EE_i^j \right| \qquad (5.4)$$

In this thesis, only parameters with $\mu^* > 0.1$ were considered significant.

## 5.3 A general framework for the selection and calibration of SST models

In wastewater treatment engineering, selection and calibration of SST models are not trivial exercises, and require a stepwise systematic approach. Here, the process of selection, calibration and validation of an SST model is described in form of a general framework (Fig. 5.1). This framework can be complementary to the good modelling practice (GMP) report recently published by the relevant Task group in the International Water Association, IWA (Rieger et al., 2012). The GMP report aims at promoting good modelling practice in activated sludge modelling by providing guidelines to select, set up, calibrate and validate the ASM-type models. However, the GMP report only gives a brief guideline for SST models selection. The steps of the proposed framework are explained in details as follows.

### 5.3.1 Engineering objective

In wastewater treatment engineering, the objective of simulating an SST behaviour using mathematical models comprise SST design (preliminary, detailed assessment); trouble-shooting of existing SSTs; sizing bioreactors combined with SST; wastewater treatment plant (WWTP) modelling; or decision, support, and control of WWTPs.

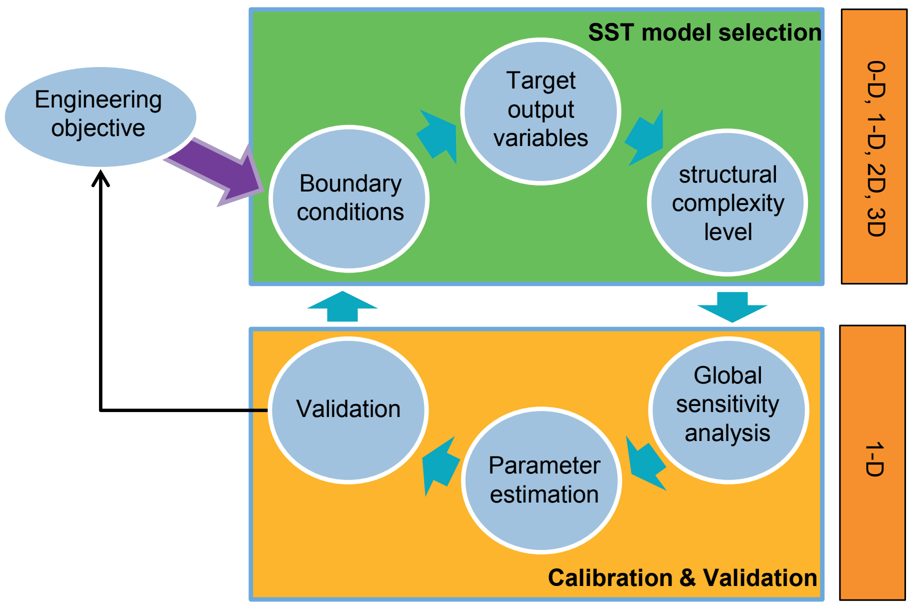


**Figure 5.1** A general framework for the selection, calibration and validation of SST models.

### 5.3.2 SST model selection

*Boundary conditions*

Depending on the engineering objective, the boundary of the SST system is specified in terms of design, flow-rate conditions, and settling characteristics. The design boundary can be described as simple (surface and depth of SST) or more detailed (also the inner structure of SST and sludge collection mechanism). Idealised flow and settling conditions are typically used for WWTP design purposes. On the other hand, for model-based WWTP optimisation objectives, plausible and realistic operational scenarios (e.g., wet-weather and bulking events) may be considered (Plósz et al., 2012).

*Target output variables*

After determining the boundary conditions, the target outputs of the SST model are determined. For the SST models used in WWTP simulations and control purposes, the sludge concentration in the effluent and recycle flow, and sludge blanket height (SBH) is sufficient to determine the sludge inventory in the system. For more detailed evaluation of the SST behaviour, the radial velocity, sheer rate, turbulent viscosity, solids viscosity profiles, stream functions and velocity vectors, and/or particle size distribution need to be additionally predicted.

*Structural complexity level*

Based on the selected boundary conditions and the target output variable requirements of a specific engineering objective, a suitable SST model complexity level needs to be selected. The complexity of the SST model is defined based on the assumptions and simplifications made in terms of space dimension (zero-, 1-D, 2-D, 3-D) and description of the hydrodynamic processes (advection, gravity settling, dispersion, flocculation, turbulence, etc.).

For WWTP models, requiring the simulation of SST in combination with bioreactors, depending on the specific engineering objective, predominantly, zero- or 1-D models are used. Zero dimensional models are formulated based on the overall mass-balance of solids around the settler and are mostly used for relatively constant flow boundary conditions (Rieger et al., 2012). 1-D SST models (section 4.1), on the other hand, can give reasonable prediction of sludge blanket dynamics in the tank, particularly in case of solids shifts from the bioreactors during high loading events. In WWTP modelling, the 1-D SST models can be coupled with the ASM-type models (Henze et al., 2000) in ordinary differential equation form by dividing the tank volume into finite number of horizontal layers.

More complex 2-D and 3-D SST models (section 4.2) are based on the mass and momentum conservation and are used for detailed design and trouble-shooting purposes. Furthermore, these models can be used as numerical experiments, replacing expensive field experiments, to calibrate and validate one-dimensional models under comparably wide flow boundary conditions (De Clercq, 2003; Plósz et al., 2007).

### 5.3.3 SST model calibration (1-D)

*Global sensitivity analysis (GSA)*

In the context of WWTP modelling, the SST model parameters are estimated along with the biokinetics, stoichiometric, and fractionation parameters through a hierarchy of calibrating the key WWTP processes. GSA can be used to identify parameter subsets with the highest sensitivity for the calibration of a WWTP model. For more information on the application of GSA and the methods see sections 5.1 and 5.2.

*Parameter estimation*

The estimation of model parameters is performed through an iterative process where the parameter values are adjusted until the difference between model predictions and measured data are within the acceptable error range. This process is optimized by adjusting only the influential parameters identified by means of GSA in the previous step and the rest are set to the default values in the model or values suggested in literature. As also recommended by the GMP protocol (Rieger et al., 2012), it is preferable to use measured values for the measurable parameters (e.g. hindered settling parameters), if the measurable parameter values need to be adjusted, it must be assured that the values are within the realistic range.

*Validation*

To complete the process of SST modelling, the models are validated by confronting them to a new set of measured data different from the ones used for model calibration. This process is also referred to as model falsification (Gernaey et al., 2004; Beven, 2008), in a sense that the model cannot be a true and valid representation of a system under any condition; it can rather survive a series of tests to describe the system within its capacity and with a reasonable accuracy. The CFD models can also be used to generate scenarios for the validation of 1-D SST models.

## 5.4 Influence of 1-D SST model selection on the calibration of WWTP models

As mentioned earlier, the current WWTP model calibration practice has most focus on the calibration of the biokinetic parameters. The uncertainties in settling parameters are often excluded from the GSA studies on WWTP models (e.g. Sin et al., 2011; Cosenza et al., 2013a; Sweetapple et al., 2013). In these studies, the first-order 1-D SST models are used and the settling parameters are set to default values so that the settling process poses no problem.

The calibration protocols, such as the GMP (Rieger et al., 2012) or the BIOMATH (Sin, 2004), recommend using measured values of settling parameters for WWTP model calibration. However, as demonstrated by Plósz et al., (2011), using measured parameter values in the first-order SST models would deteriorate their prediction of sludge inventory in the system. It was argued that settling parameters in first-order SST models are in fact lumped model parameters that are fine-tuned (sometimes to unrealistic values) during the calibration procedure to compensate for the uncertainty propagating from the mathematical structure of the model. In fact, as stated by Krebs (1995), it is always possible to find a best fit with the first-order 1-D SST models by fine-tuning the settling parameters. In the second-order 1-D SST modelling approach, the explicit dispersion term lumps all the hydrodynamic features in the tank that cannot be described in one dimension (Ekama et al., 1997). Therefore, the second-order models allow for clear distinction between settling parameters, which are measurable, and other lumped SST model parameters, which require adjustment during model calibration. Due to differences in the model structure, the first and second order 1-D SST models require different settings for their parameter values and consequently selecting either of them would influence the calibration of WWTP models.

These concerns has been address in **Paper I** of this thesis (Ramin et al., 2014). This study investigated the influence of selecting the first-order and second-order 1-D SST modelling approaches on the optimum parameter selection for the calibration of WWTP models, particularly for predicting biogas production and treated water quality. GSA was performed on BSM2 with the first-order 1-D SST model by Takács et al. (1991) and the second-order 1-D SST model by Plósz et al. (2007). The input uncertainty consisted of the fractionation and biokinetic parameters, as well as the settling parameters. The GSA methods applied were linear regression of Monte Carlo simulations and Morris Screening to independently cross-check the validity of the sensitivity measures.

Based on most of the parameter sensitivity rankings obtained in this study (Figs 3 and 4 in **Paper I**), the settling parameters were found to be as influential as the biokinetic parameters on the uncertainty of plant model predictions. This was found from the GSA results of the two simulation scenarios regardless of the SST model structure. This means that the calibration of WWTP models should give equal importance to estimation of the settling parameters and biokinetic parameters. Moreover, it was found that the SST model selection influences the importance ranking of the settling parameters. From the GSA on simulation scenarios using the first-order SST model, most of the BSM2 model outputs were found to be equally sensitive to the hindered settling parameters ($r_H$ and $v_0$) and $r_P$ (in Eq.3.2). In contrast, in case of using the second-order SST model, the significance of $r_P$ was obtained to be much less than $r_H$ and $v_0$ and for some model outputs even insignificant. An example of the GSA results for methane production is illustrated in Fig. 5.2. The difference in the sensitivity measure of $r_p$ using the first- and the second-order 1-D SST models is pointed in the rankings with the dotted ellipse.

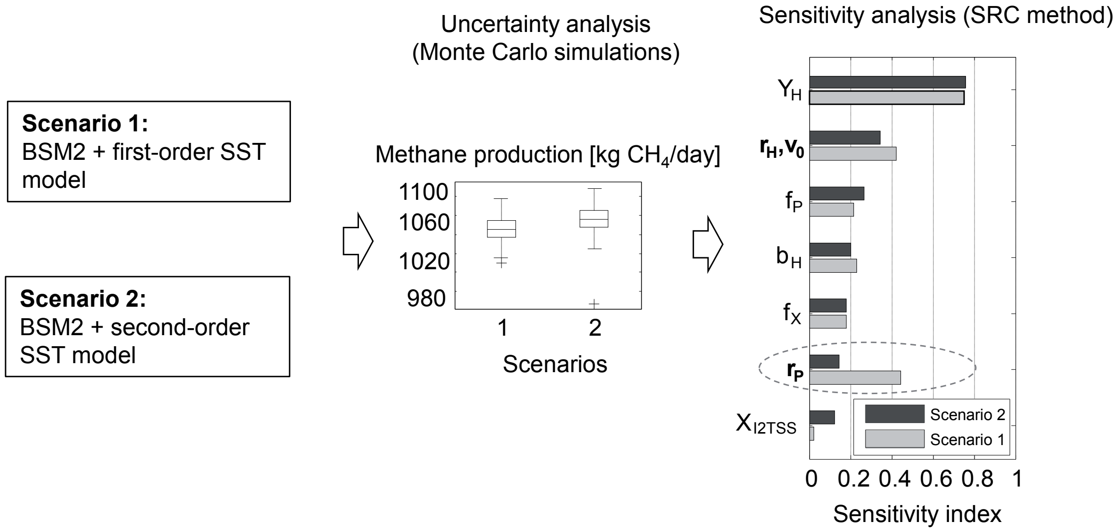


**Figure 5.2** A schematic of the GSA results in Paper I in identifying the influential parameters to the variance of WWTP model outputs, with an example on methane production (**Paper I**).

These results advocate the advantage of using second-order models in order to perform calibrations in line with the good modelling practice proposed by the GMP protocol (Rieger et al., 2012).

## 5.5 Significance of 1-D SST model structures and parameter subsets under wet-weather flow and filamentous bulking conditions

In the second GSA study of this thesis (**Paper II**), the aim was to supplement the GMP report with practical findings on the calibration of 1-D SST models for dynamic WWTP simulations under different flow and settling boundary conditions. In this regard, a comparative evaluation of the first- and second-order 1-D SST models in WWTP simulations under ideal and non-ideal/realistic flow (dry- and wet-weather) and settling (good settling or bulking) boundary conditions was performed by means of GSA.

The results illustrated that the contribution of settling parameters to the total variance of the key WWTP process outputs greatly depends on the influent flow and settling conditions. For instance, the change from dry- to wet-weather inflow rate under good settling condition increases the significance of $r_P$. However, imposing bulking condition significantly adds to the influence of hindered settling parameters ($r_H$ and $v_0$).

The impact of boundary conditions on the identified parameter subsets depended on the 1-D SST model selected. For example, the influence of the change in the WWTP inflow rate on the significance of $r_P$ was more evident when using the first-order 1-D SST model. On the other hand, under bulking conditions, the sensitivity of the WWTP model outputs to the hindered settling parameters is comparably higher when using the second-order 1-D SST model. These results encourage the use of second-order 1-D SST models for dynamic WWTP simulations under a wide range of flow and settling conditions, where the measurable hindered parameters play an important role in model calibration.

Finally, temporal evaluation of the sensitivity measures of the second-order SST model parameters under wet-weather flow conditions revealed the hydraulic parameters in the second-order SST model become a high source of uncertainty during wet-weather flow conditions. Fig. 5.3a shows an example of the contribution of settling parameters to the sludge inventory and secondary settling related outputs. Fig. 5.3b shows the temporal change in the sensitivity of the hydraulic parameter ($v_{OV,DIS}$) under wet-weather flow variations for the prediction of sludge blanket height. This result highlights the importance of developing a more mechanistic flow-dependent hydraulic sub-model in second-order SST models in the future.

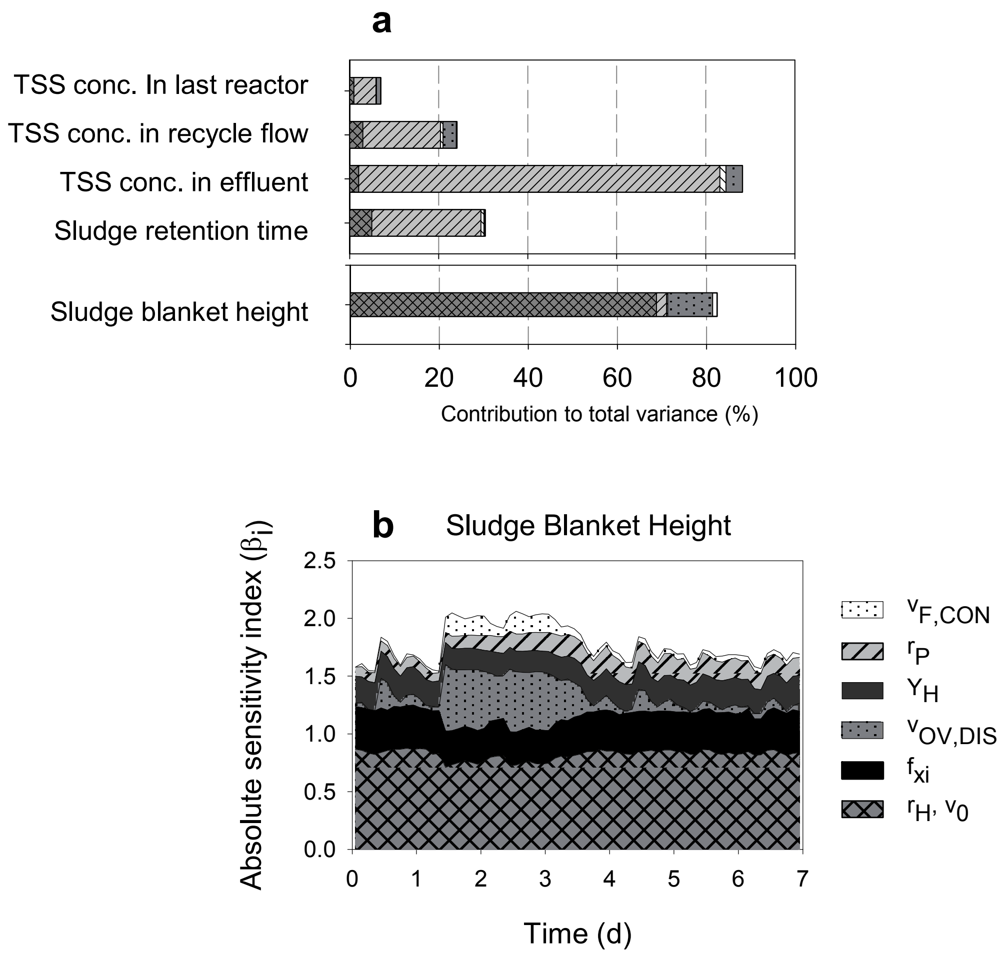


**Figure 5.3** Total contribution of settling parameters to the sensitivity of model outputs related to the sludge inventory and secondary settling processes in WWTPs (**a**), and an example of temporal evolution of sensitivity measures of significant parameters under wet-weather flow variations for the prediction of sludge blanket height (**b**). (**Paper II**)

# 6 CFD model development

As previously outlined, the validated CFD models are effective tools in describing the flow behaviour of the system. Moreover, the optimized CFD model are potential tools to develop a more mechanistic based flow (and design) dependent hydraulic sub-model in the second-order 1-D SST models.

The current CFD models are mostly optimized in terms of modelling the turbulence, and buoyant flow components, and, to some extent, the models describing the rheological behaviour of activated sludge under the shear conditions in the SSTs. However, regarding the settling sub-model, the empirical settling velocity function of Takács et al. (1991) is widely used in the CFD models. Takács settling function only describes the hindered and slow settling regimes, whereas the application of the recently developed mechanistic compression settling velocity models (section 3.2) are only limited to a few case of 1-D SST modelling (De Clercq et al., 2008; Bürger et al., 2011, 2012, 2013).

The settling process in the CFD domain can also be modelled as a 1-D process by identifying a settling velocity model based on observations n batch settling experiments. However, the calibration of models accounting for compression settling, requires dynamic monitoring of sludge profiles in batch settling experiments, and is not simple in practice.

## 6.1 A new settling velocity and rheology model for CFD modelling of SSTs

Based on the above mentioned motivations, the third study of this thesis (**Paper III**) was dedicated to the development of a CFD model and optimization of the settling and rheology models using data from batch experiments. A simple, new settling experimental set-up was developed in this study to obtain data for the evaluation of the currently available settling velocity models, which resulted in the development of a new settling velocity model. Furthermore, rheology measurements were performed and new correlations between rheological model parameters and sludge concentration were established.

### 6.1.1 Identifying a new settling velocity model

The new settling experimental set-up consisted of a large glass column (D = 20 cm, H = 80 cm) with a Solitax® TSS sensor installed at the bottom of the column to record the evolution of sludge accumulation at the bottom. Two sets of experiments with sludge samples from two different WWTPs were performed by diluting the samples with the SST effluent to obtain a concentration range typical for the feed flow to the SSTs (1.7 – 5 g/l). During each test, the *SBH* and bottom sludge concentration ($X_b$) were measured.

To evaluate the state-of-the-art settling velocity models against the batch measurements, a 1-D model of the settling column (Plósz et al., 2007) was implemented in MATLAB®. The 1-D model of the column test is a discretised form of a mass conservation partial differential equation, including 60 horizontal layers along the depth of the column (similar to 1-D SST model described in section 4.1). To estimate the settling velocity model parameters, the 1-D model was coupled with the $DREAM_{ZS}$ optimization algorithm (see section 3.4). The Bayesian approach, as compared to the classical optimization methods, provides more information on the uncertainty of model parameters by calculating the posterior parameter distributions (Eq. 3.5).

Based on the evaluation of different settling functions, a new settling velocity function (Eq. 6.1) was developed, which could very accurately predict the measured *SBH* and $X_b$ time-series (Fig. 6.1):

$$v_S = \begin{cases} v_0 e^{-r_H . X} - v_0 e^{-r_P . X} & X < X_C \\ v_{0,t} e^{-r_t X} \left(1 - \dfrac{\rho_S}{(\rho_S - \rho_f) g X} \left(\dfrac{X - X_C}{C_1}\right)^{C_2} \dfrac{dX}{dz}\right) & X \geq X_C \end{cases} \tag{6.1}$$

where $v_0$ is the ultimate settling velocity; $r_H$ and $r_P$ are the hindered and low concentration settling characteristic indices, respectively; $\rho_s$ and $\rho_f$ are the sludge and water density, respectively; $g$ denotes the gravity constant; $X$ is the sludge concentration at depth $z$ of the column; $X_C$ is the compression threshold concentration; $C_1$ and $C_2$ are the compression parameters.

In Fig. 6.1 the prediction accuracy of the new settling velocity model is demonstrated by applying it to a 1-D model of a settling column and calibrating it simultaneously to the *SBH* and $X_b$ measurements. The predictive uncertainty of the new settling velocity model calibrated to all the measured settling curves with the sludge from Lundtofte WWTP is shown in Fig. 6.2.

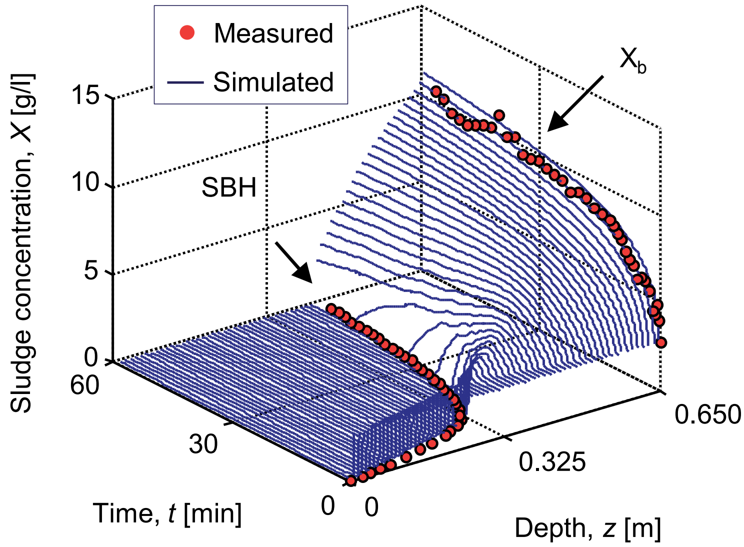


**Figure 6.1** Prediction of the new settling velocity model calibrated to the *SBH* and $X_b$ measurements by implementing it to a 1-D settling column model (60 layers discretization). The lines correspond to the simulated evolution of the sludge concentration in each layer. (**Paper III**)

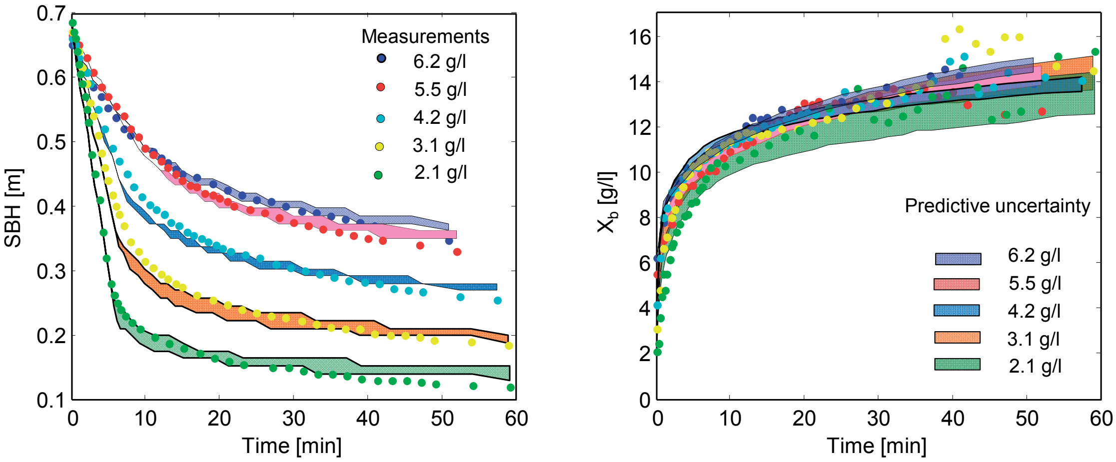


**Figure 6.2** Predictive uncertainty (95% confidence intervals of the model prediction due to parameter uncertainty) of the new velocity model calibrated to the measurements with the Lundtofte WWTP sludge using DREAM$_{(ZS)}$ optimization algorithm. (**Paper III**)

## 6.1.2 Identifying new rheological correlations

The rheological measurements obtained with a rotational rheometer (Fig. 6.3a) on the sampled sludge from Lundtofte WWTP, revealed a pseudo-plastic behaviour of sludge with yield stress (Fig. 5.3b). The Herschel-Bulkely rheology sub-model was selected and calibrated to the measurements (Fig. 6.3b):

$$\tau = \tau_0 + K\gamma^n \tag{6.2}$$

where $\tau_0$ is the yield stress, $K$ is the consistency index, and $n$ is the flow behaviour index.

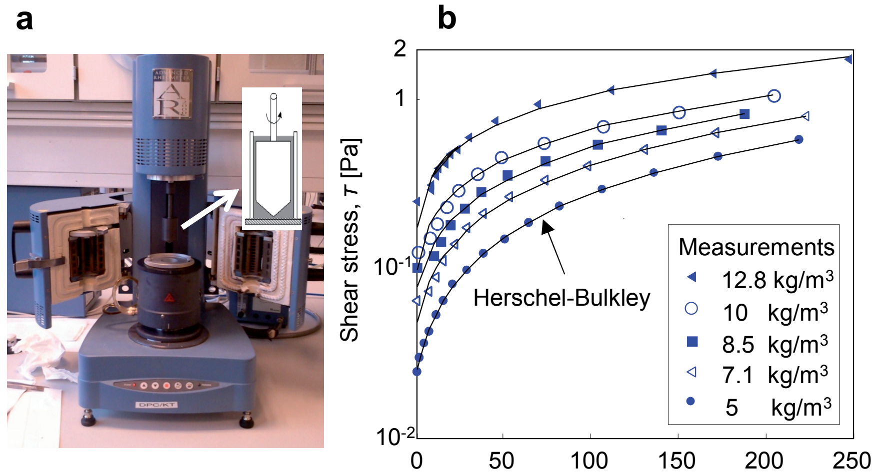


**Figure 6.3** Rheological measurements (**a**) for selection and calibration of the Herschel-Bulkely rheology model **(b)**

The estimated parameters of the Herschel-Bulkley model were found to be strongly dependent on sludge concentration. Therefore, three new correlations between the parameters and sludge concentration were established:

$$\tau_0 = AX^B \tag{6.3}$$

$$K = \eta_w e^{C.X} \tag{6.4}$$

$$n = \frac{1}{1 + DX^E} \tag{6.5}$$

where $A$, $B$, $C$, $D$, and $E$ are rheological correlation parameters.

### 6.1.3 CFD simulations

The circular conical centre-feed SST at Lundtofte WWTP was simulated with a CFD model developed in OpenFOAM®. The hydrodynamics of the solver is based on the averaged form of the Eulerian two-phase flow (section 4.2.1). The turbulence was modelled with the buoyancy modified *k*-*ε* model (section 4.2.2). The new settling velocity model and rheology correlations were implemented in the CFD model with parameter values estimated from batch settling experiments (sections 6.1.1 and 6.1.2).

The flow pattern in the tank predicted with the CFD model was in close agreement with the flow field captured by the velocity profile measurements (Fig. 6.4).

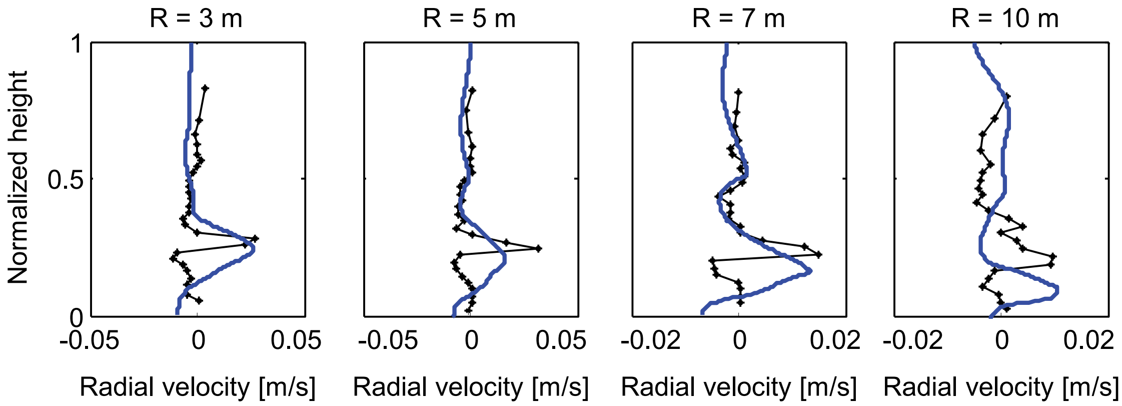


**Figure 6.4** Predicted velocity profiles (solid lines) at four different radial distances from the centre of SST against measured profiles (marked lines). (**Paper III**)

The strong density current can be observed in Fig 6.5 just above the sludge blanket (Fig. 6.5a). It can be observed in Fig 6.5b how the turbulence is damped by the viscous sludge in the vicinity of sludge blanket.

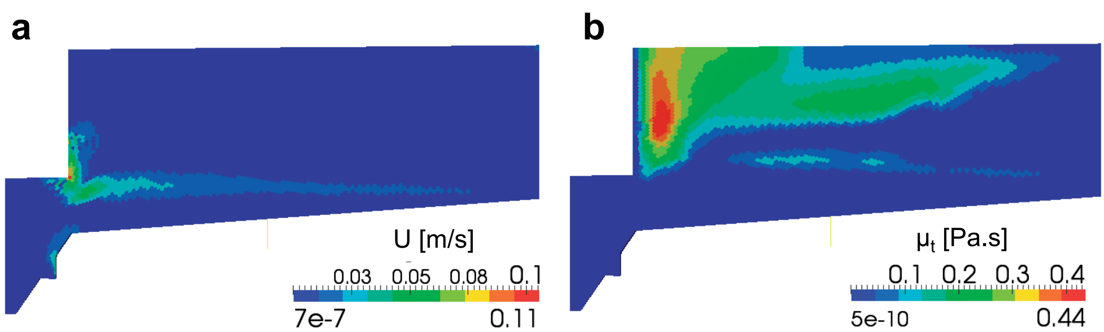


**Figure 6.5** The CFD predicted velocity (**a**), and turbulent viscosity (**b**) in the SST under study at Lundtofte WWTP. (**Paper III**)

### 6.1.4 CFD predictions with the new settling velocity model

It was further assessed whether the presence of the compression settling velocity model in the CFD model influences the prediction of sludge distribution. In this regards, the CFD predictions using the new settling velocity model was compared with the ones using the widely used Takács hindered settling velocity model against the measured profiles. Fig. 6.6 clearly indicates the improvement of the CFD model predictions in terms of sludge distribution using the new settling velocity function. Only the profiles at 7m radial distance from the tank centre are shown in Fig. 6.6; for full comparison the reader is referred to Fig. 6 in **Paper III**.

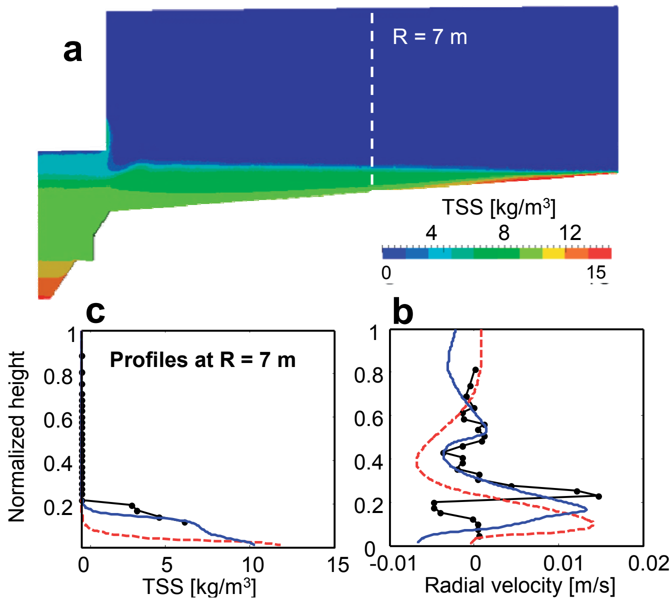


**Figure 6.6** Predicted sludge distribution in the Lundtofte SST using the new settling velocity model (**a**), a vertical profile (normalized height) of sludge concentration $X$ (**b**), and the radial velocity (**c**) at 7 m radial distance from the tank centre. Measurements (thin marked lines), CFD model predictions with the new settling velocity model (solid blue line), and CFD model predictions using Takács settling velocity model (dashed red line).

In summary, the settling velocity function developed in this study is shown to significantly improve the prediction accuracy of the CFD models in terms of sludge distribution, as compared to the widely used Takács settling function. Moreover, the new settling function can be used explicitly in the 1-D SST models. The simple settling experiments combined with a Bayesian optimization approach can replace the extensive profiling experiments, e.g. radiotracer tests (De Clercq et al., 2005), to calibrate the new settling velocity function and account for transient, hindered and compression settling regimes in numerical modelling of SSTs.

# 7 Conclusions

1-D SST models with first- and second-order equation types are used in combination with ASM-type models for dynamic simulation of WWTPs. Despite the limitations in their application, as compared to the second-order SST models, the first-order models are still widely used. The aim of this thesis was to direct the current WWTP modelling practice towards the application of the more mechanistic second-order 1-D SST models by evaluating their significance using global sensitivity analysis (GSA). Moreover, laboratory and numerical tools were developed to identify and calibrate the sub-models in the SST models.

Firstly, this thesis aimed to assess the significance of SST model selection for WWTP simulations by means of GSA. The settling parameters were found to be as influential on the uncertainty of WWTP model predictions as the biokinetic parameters. Importantly, the choice of 1-D SST models was shown to significantly influence the overall performance of WWTP models. The sensitivity of WWTP model outputs to the model parameters was found to be dependent on the 1-D SST models selected. Accordingly, different optimum parameter selection for the calibration of WWTP models was suggested when using each of the 1-D SST models. Only the procedure required for the calibration of the second-order SST models was found to be in close agreement with the recommendations made in the Good Modelling Practice protocol on activated sludge modelling.

Secondly, a GSA study on the WWTP models under ideal and realistic flow and settling conditions revealed that the sensitivity of WWTP model outputs to the 1-D SST mod parameters (being first- or second-order SST model) strongly depends on the imposed boundary conditions, resulting in different parameter subsets for the WWTP model calibration. Moreover, it was found that the impact of boundary conditions on the identified parameter subsets depends on the 1-D SST model selected. The results advocate the use of second-order SST models for dynamic WWTP simulations under a wide range of flow and settling conditions, where the measurable hindered parameters play an important role in model calibration. Importantly, the hydraulic parameters in the second-order SST model become a high source of uncertainty during wet-weather flow conditions. Hence, these results highlight the importance of developing a more mechanistic flow-dependent hydraulic sub-model in second-order SST models in the future.

Thirdly, an optimized CFD model of an SST including new settling velocity and rheological models was developed. The CFD model was shown to predict the full-scale measurements with overall high accuracy. The new settling velocity model developed in this study accurately described the hindered, transient and compression settling regimes observed in the batch experiments. Furthermore, the model significantly improved the sludge distribution prediction accuracy of the CFD models when compared to models employing the widely used Takács settling model. The validated CFD model was also used to model the impact of filamentous bulking on the sludge distribution and transport in SSTs. CFD scenario simulations where performed by calibrating the rheology and settling models with the data obtained from experiments with sludge of high and low filamentous content.

In summary, developing effective numerical tools to predict and mitigate the impact of high hydraulic loadings on the performance of SSTs can subsequently be used to estimate the hydraulic capacity of SSTs and decrease the amount of sewage by-passing in WWPTs under wet-weather conditions.

*Implication of the results on future WWTP simulation studies*

This thesis provided practical findings on the calibration of first- and second-order 1-D SST models for WWTP simulations. The parameter sub-sets were identified for WWTP model calibrations with 1-D SST models under ideal and realistic flow and settling boundary conditions. These results complement the GMP protocol and can be used in the common WWTP modelling practice.

*Implication of the results on the future developments of more mechanistic second-order 1-D SST models*

The optimized CFD model developed in this study can be used as a tool to develop more mechanistic based flow (and design) dependent hydraulic sub-models in the second-order 1-D SST models, with the help of tools such as dimensional analysis and experimental design methodologies.

The new settling velocity model developed in this thesis can be used explicitly in the 1-D SST models. The proposed simple experimental methodology, combined with the efficient Bayesian optimization algorithm $DREAM_{(ZS)}$, enables the application of the new settling velocity model for on-line control purposes.

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# 9 Papers

I **Ramin, E.**, Flores Alsina, X., Sin, G., Gernaey, K.V., Jeppsson, U., Mikkelsen, P.S., and Plósz, B.G. (2014). Influence of selecting secondary settling tank sub-models on the calibration of WWTP models – A global sensitivity analysis using BSM2. *Chemical Engineering Journal*. **241**: 28-34.

II **Ramin, E.**, Sin, G., Mikkelsen, P.S., and Plósz, B.G. (2014). Significance of settling model structures and parameter subsets in modelling WWTPs under wet-weather flow and filamentous bulking conditions. *Submitted manuscript*.

III **Ramin, E.**, Wágner, D.S., Yde, L., Binning, P.J., Rasmussen, M.R., Mikkelsen, P.S., and Plósz, B.G. (2014). A new settling velocity and rheological model for secondary settling tank modelling. *Submitted manuscript*.

IV **Ramin, E.**, Wágner, D.S., Szabo, P., Dechesne, A., Smets, B.F, and Plósz, B.G. (2014). Impact of filamentous microbial community characteristics on activated sludge settling and rheological behaviour – measurements and numerical modelling. *Manuscript in preparation*.

In this online version of the thesis, the articles are not included but can be obtained from electronic article databases e.g. via www.orbit.dtu.dk or on request from.

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The Department of Environmental Engineering (DTU Environment) conducts science-based engineering research within four sections:
Water Resources Engineering, Urban Water Engineering,
Residual Resource Engineering and Environmental Chemistry & Microbiology.

The department dates back to 1865, when Ludvig August Colding, the founder of the department, gave the first lecture on sanitary engineering as response to the cholera epidemics in Copenhagen in the late 1800s.

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